

Supporting Information for

Highly Stable Organic Bisradicals Protected by Mechanical Bonds

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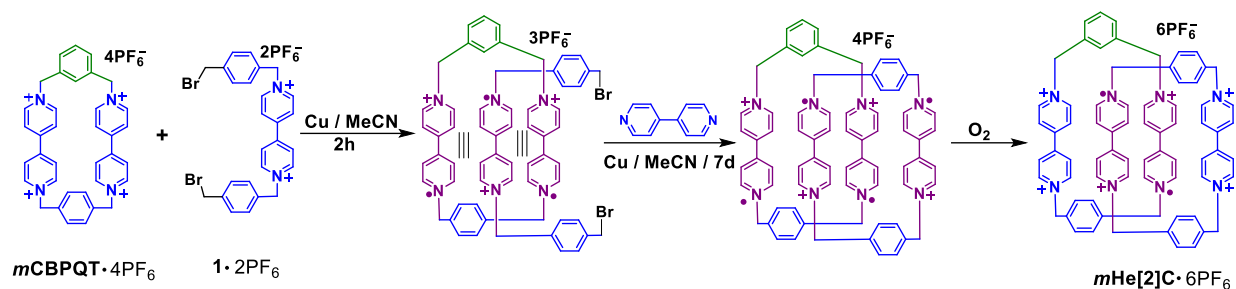
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Section A. General Methods

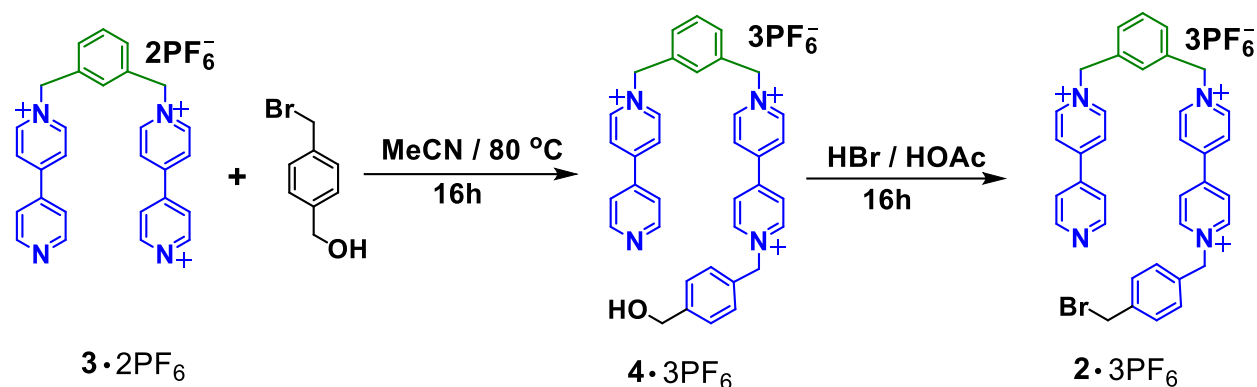
All reagents were purchased from commercial suppliers and used without further purification. Compounds **1**•2PF₆, **CBPQT**•4PF₆, **mCBPQT**•4PF₆ were prepared^{S1} according to literature procedures. Thin layer chromatography (TLC) was performed on silica gel 60 F254 (E. Merck). Column chromatography was carried out on silica gel 60F (Merck 9385, 0.040–0.063 mm). C-18 Columns were used for analytical and preparative reverse-phase high-performance liquid-chromatography (RP-HPLC) on Agilent 1260 infinity LC equipped with Agilent 6120 LC/MS electrospray system and Shimadzu Prominence LC-8a instruments, respectively, eluted with H₂O/MeCN (0.1 % v/v TFA) and monitored using a UV detector (λ = 360 nm). UV/Vis Spectra were recorded at room temperature on a Shimadzu UV-3600 spectrophotometer. Nuclear magnetic resonance (NMR) spectra are recorded on Agilent DD2 500 as well as on Bruker Avance III 400 and 500 spectrometers, with working frequencies of 400 and 500 MHz for ¹H, as well as 100 and 125 MHz for ¹³C nuclei, respectively. Chemical shifts were reported in ppm relative to the signals corresponding to the residual non-deuterated solvents (CD₃CN: δ_{H} = 1.94 ppm and δ_{C} = 118.26 ppm for ¹³CN). High-resolution mass spectra (HR-ESI) were measured on a Finnigan LCQ iontrap mass spectrometer. Electron paramagnetic resonance (EPR) measurements at X-band (9.5 GHz) were performed with a Bruker Eleksys E580, equipped with a 4122SHQE resonator. All samples were prepared in an Argon-filled atmosphere. Scans were performed with magnetic field modulation amplitude of 1 G and non-saturating microwave power between 0.4 and 0.6 mW. Samples were contained in quartz tubes with I.D. 1.50 mm and O.D. 1.80 mm and sealed with a clear ridged UV curin epoxy (IllumaBond 60-7160RCL) and used immediately after preparation. Cyclic voltammetry (CV) and differential pulse voltammetry (DPV) experiments were carried out at room temperature in Argon-purged MeCN solutions with a Gamry Multipurpose instrument (Reference 600) interfaced to a PC. CV Experiments were performed using a glassy carbon working electrode (0.071 cm²). The electrode surface was polished routinely with 0.05 μ m alumina-water slurry on a felt surface immediately before use. The counter electrode was a Pt coil and the reference electrode was Ag/AgCl electrode. The concentration of the supporting electrolyte tetrabutylammonium hexafluorophosphate (NH₄PF₆) was 0.1 M.

Section B. Synthetic Protocols



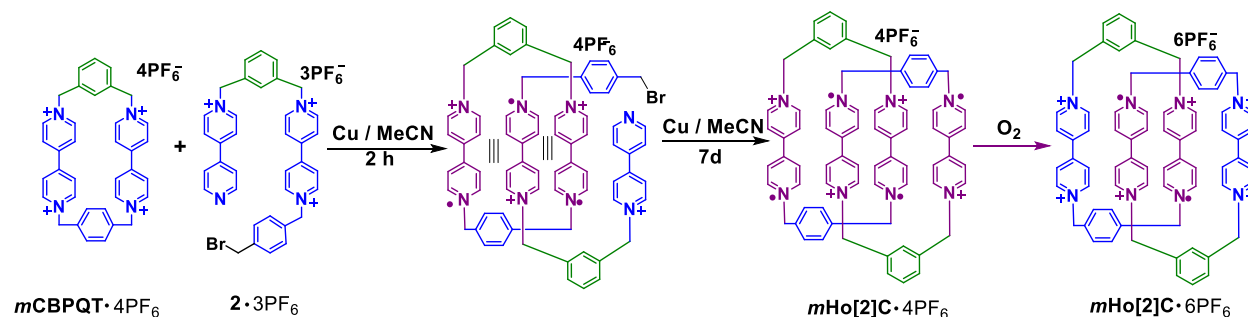
$m\text{He}[2]\text{C}\cdot 6\text{PF}_6$: $m\text{CBPQT}\cdot 4\text{PF}_6$ (330 mg, 0.30 mmol) and $1\cdot 2\text{PF}_6$ (270 mg, 0.34 mmol) were dissolved in degassed MeCN (60 mL) in a 100-mL round-bottomed flask in a N_2 -filled glovebox. An excess of Cu dust (~100 mg) was added with stirring to this solution. After 2 h, the solution turned from colorless to a deep purple color, an observation which is indicative of the formation of the trisradical tricationic complex. Then 4,4'-bipyridine (54 mg, 0.34 mmol) was added to it, and the resulting mixture was allowed to stand for 7 days at room temperature. Cu Dust was removed by filtration and the solvent was evaporated off under vacuum. The crude product was purified using reversed-phase flash chromatography (C_{18} : $\text{H}_2\text{O}/\text{MeCN}$ 0.1% TFA 0-100%), followed using anion exchange from TFA^- to PF_6^- by treating the aqueous fractions with an excess of NH_4PF_6 , resulting in a white precipitate which was collected by centrifugation and washed with H_2O several times before being dried *in vacuo* to afford $m\text{He}[2]\text{C}\cdot 6\text{PF}_6$ as a dark purple solid (170 mg, 30%). For NMR spectroscopic characterization, $m\text{He}[2]\text{C}\cdot 6\text{PF}_6$ (2 mg) was oxidized to $m\text{He}[2]\text{C}\cdot 8\text{PF}_6$ by the addition of an excess (1 mg) of $\text{NO}\cdot\text{PF}_6$. ^1H NMR (500 MHz, CD_3CN , 298 K) of $m\text{He}[2]\text{C}\cdot 8\text{PF}_6$: δ 9.03 (d, $J = 6.6$, 6H), 8.99 (d, $J = 7.0$ Hz, 2H), 8.87 (d, $J = 6.6$ Hz, 2H), 8.83 (d, $J = 6.6$ Hz, 2H), 8.72 (d, $J = 6.0$ Hz, 2H), 8.40 (s, br, 1H), 8.34-8.32 (m, 4H), 8.17 (d, $J = 7.0$ Hz, 2H), 8.14 (s, br, 9H), 8.06 (s, br, 2H), 7.85 (d, $J = 6.5$ Hz, 2H), 7.79 (d, $J = 6.5$ Hz, 4H), 7.74 (d, $J = 6.5$ Hz, 2H), 6.17-6.13 (m, 6H), 6.00-5.96 (m, 10H), 5.09 (s, br, 2H), 4.28-4.22 (m,

6H). ^{13}C NMR (125 MHz, CD_3CN , 298 K) of $m\text{He}[\mathbf{2}]\text{C}\cdot 8\text{PF}_6$: δ 149.0, 148.8, 148.3, 148.0, 147.7, 147.3, 146.9, 146.6, 143.4, 143.2, 142.8, 140.4, 140.0, 138.8, 138.2, 136.9, 136.8, 135.8, 135.1, 134.7, 133.0, 132.9, 132.5, 132.0, 128.2, 128.0, 127.7, 122.9, 122.9, 122.5, 67.5, 67.2, 67.0, 65.6, 65.5, 65.4. ESI-HRMS for $m\text{He}[\mathbf{2}]\text{C}\cdot 6\text{PF}_6$; Calcd for $\text{C}_{72}\text{H}_{64}\text{F}_{36}\text{N}_8\text{P}_6$: $m/z = 810.1905$ [$M - 2\text{PF}_6$] $^{2+}$; found: 810.1889.



4•3PF₆: **3•2PF₆** (350 mg, 0.50 mmol) and (4-(bromomethyl)phenyl)methanol (120 mg, 0.60 mmol) were dissolved in degassed MeCN (60 mL) in a 100-mL round-bottomed flask. The solution was heated to 80 °C for 16 h with stirring. After cooling down to room temp, excess of TBACl was added to the solution. The solids were collected by filtration, and the crude product was purified by reversed-phase flash chromatography (C_{18} : $\text{H}_2\text{O}/\text{MeCN}$ 0.1% TFA 0-100%), followed by anion exchange from TFA^- to PF_6^- by treating the aqueous fractions with an excess of NH_4PF_6 , resulting in a white precipitate which was collected by centrifugation and washed with H_2O several times before being dried *in vacuo* to afford **4•3PF₆** as an off-white solid (211 mg, 45%). ^1H NMR (500 MHz, CD_3CN , 298 K): δ 9.00-8.94 (m, 8H), 8.42-8.37 (m, 8H), 7.63-7.59 (m, 4H), 7.59 (s, 4H), 5.87-5.85 (m, 4H), 5.83 (s, 2H), 4.65 (s, 2H). ^{13}C NMR (125 MHz, CD_3CN , 298 K) δ 151.9, 151.4, 151.0, 146.5, 146.4, 145.2, 143.9, 134.7, 132.0, 131.6, 131.6, 131.3, 130.2, 128.44, 128.42, 128.36, 128.32, 127.4, 100.8, 65.4, 64.9, 64.8.

2•3PF₆: **4•2PF₆** (160 mg, 0.83 mmol) was dissolved in HBr (33% in HOAc) (10 mL) in a 25-mL vial. The solution stirred under rt for 16 before the all the solvents were removed *in vacuo*. The residue was dissolved in water (10 mL), and excess NH₄PF₆ were added to the solution. The precipitate was collected by filtration, washed with H₂O for several times before being dried *in vacuo* to afford **2•3PF₆** as an off-white solid (153 mg, 92%). ¹H NMR (500 MHz, CD₃CN, 298 K): δ 9.00-8.93 (m, 8H), 8.41-8.38 (m, 8H), 7.64-7.50 (m, 8H), 5.85-5.84 (m, 6H), 4.654 (s, 2H). ¹³C NMR (125 MHz, CD₃CN, 298 K) δ 151.9, 151.3, 151.1, 146.5, 146.5, 145.2, 143.9, 134.7, 132.0, 131.6, 131.6, 131.3, 130.2, 128.46, 128.40, 128.35, 128.2, 127.4, 100.8, 65.4, 65.0, 63.6.



mHo[2]C•6PF₆: Following a procedure similar to that described for the synthesis of **mHe[2]C•6PF₆**, the reaction of a mixture composed of **mCBPQT•4PF₆** (220 mg, 0.20 mmol), **2•3PF₆** (142 mg, 0.17 mmol) afforded **mHo[2]C•6PF₆** as a dark purple solid (69 mg, 18%). For NMR spectroscopic characterization, **mHo[2]C•6PF₆** (2 mg) was oxidized to **mHo[2]C•8PF₆** by the addition of an excess (1 mg) of NO•PF₆. ¹H NMR (500 MHz, CD₃CN, 298 K) of **mHo[2]C•8PF₆**: δ 9.09 (d, *J* = 8.0 Hz, 2H), 9.03-9.01 (m, 4H), 8.98 (d, *J* = 7.5 Hz, 2H), 8.82 (d, *J* = 6.5 Hz, 2H), 8.76 (d, *J* = 6.5 Hz, 8H), 8.42-8.32 (m, 18H), 7.87-7.85 (m, 4H), 7.77-7.75 (m, 4H), 7.65-7.63 (m, 2H), 6.20-5.97 (m, 16H), 5.29 (s, br, 2H), 4.98 (s, br, 2H), 4.38 (s, br, 2H), 4.07 (s, br, 2H). ¹³C NMR (125 MHz, CD₃CN, 298 K) of **SC•8PF₆**: δ 148.3, 147.7, 147.5, 147.0, 146.6, 146.3, 143.3, 142.4, 142.2, 140.0, 138.6, 136.6, 136.3, 135.2, 134.5, 132.8, 131.9, 131.4, 131.0, 128.1, 127.9, 127.6, 127.3, 67.1, 66.4, 65.4, 65.3. ESI-HRMS for **mHo[2]C•6PF₆**; Calcd for C₇₂H₆₄F₃₆N₈P₆: *m/z* = 810.1905 [*M* – 2PF₆]²⁺; found: 810.1895.

Section C. NMR Spectroscopy

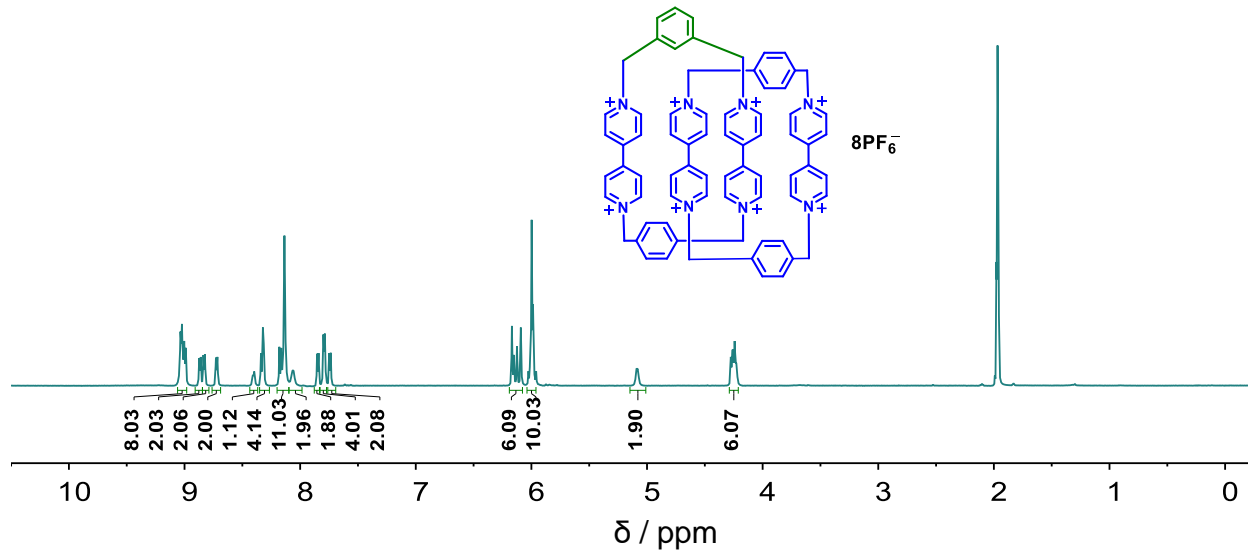


Figure S1. ^1H NMR Spectrum (500 MHz, CD_3CN , 298 K) of $m\text{He}[2]\text{C}\cdot 8\text{PF}_6$.

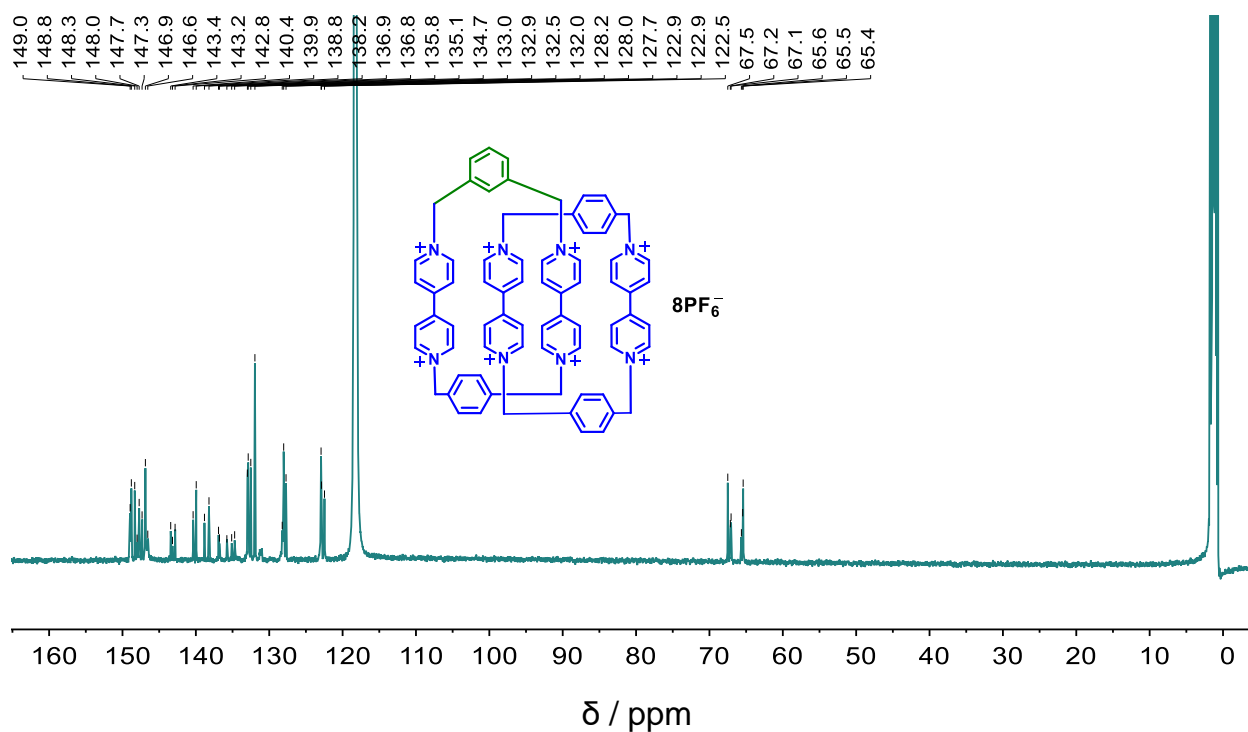


Figure S2. ^{13}C NMR Spectrum (500 MHz, CD_3CN , 298 K) of $m\text{He}[2]\text{C}\cdot 8\text{PF}_6$.

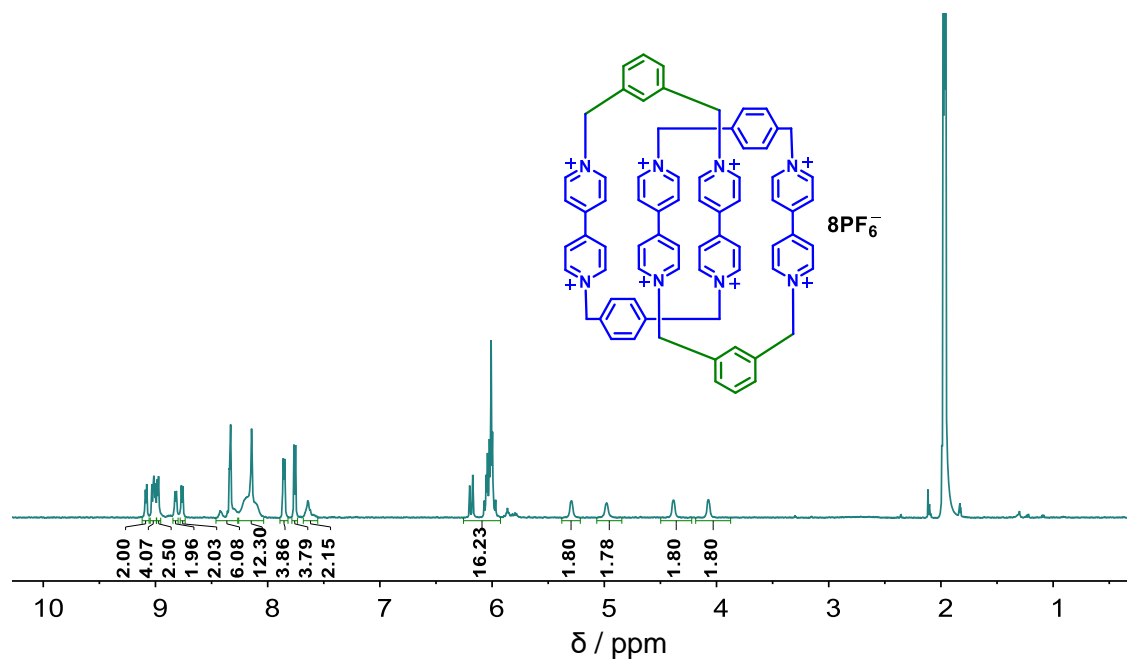


Figure S3. ^1H NMR Spectrum (500 MHz, CD_3CN , 298 K) of $m\text{Ho}[2]\text{C}\cdot 8\text{PF}_6$.

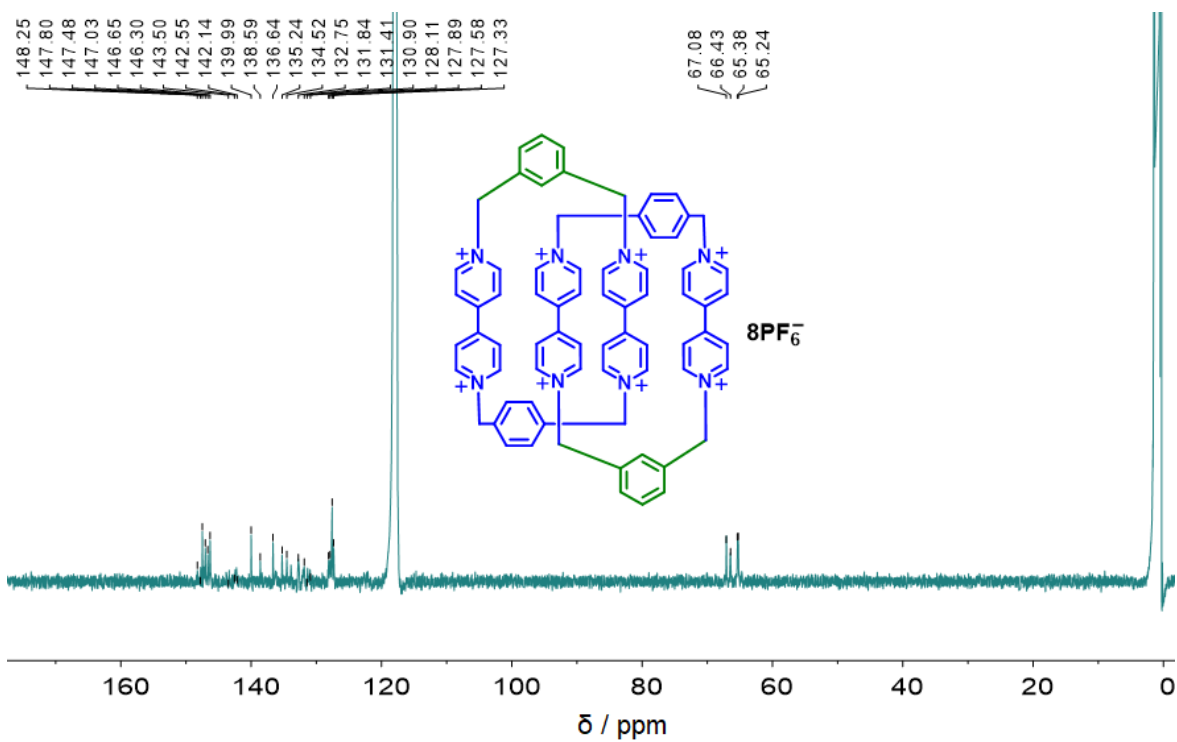


Figure S4. ^{13}C NMR Spectrum (500 MHz, CD_3CN , 298 K) of $m\text{He}[2]\text{C}\cdot 8\text{PF}_6$.

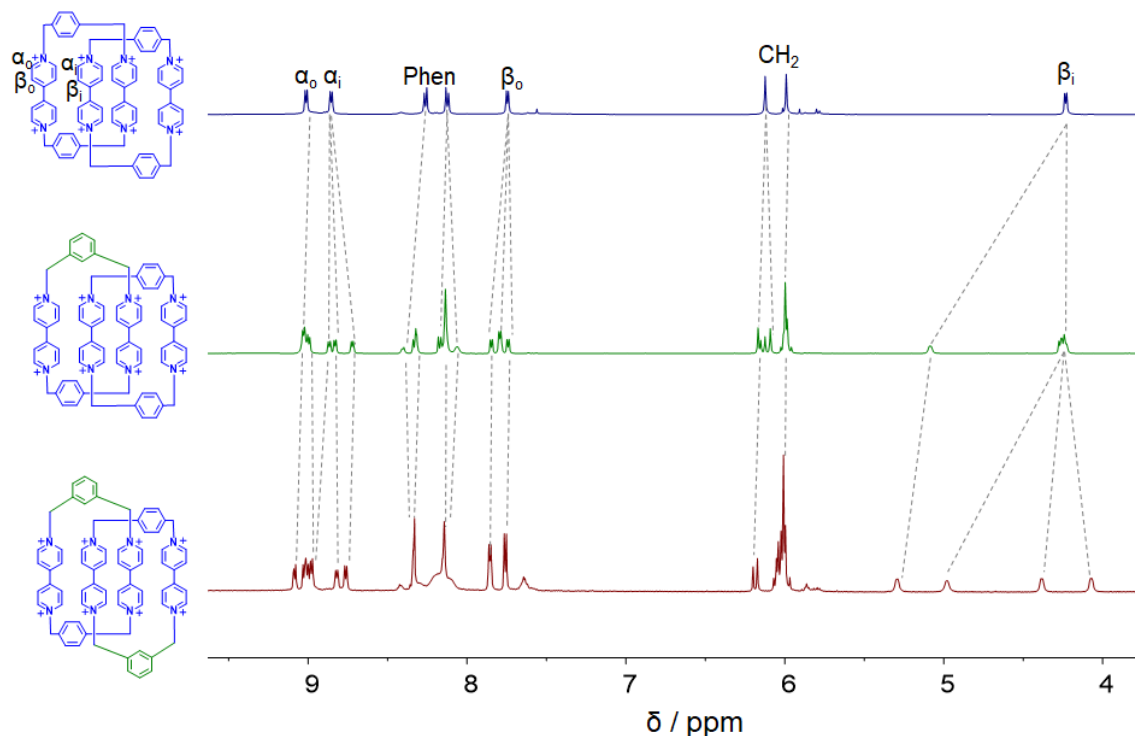


Figure S5. Stacked ^1H NMR spectra (500 MHz, CD_3CN , 298 K) of **Ho[2]C•8PF₆**, **mHe[2]C•8PF₆** and **mHo[2]C•8PF₆**.

Section D. Vis/NIR Absorption Spectroscopy

The solution of two catenanes with different redox states were prepared by employing electrochemical reductions under different potentials: **mHe[2]C•6PF₆** (6.3 mg) was dissolved in MeCN (30 mL) in a N_2 -filled glovebox. The solution was then added into the working cell, while the auxiliary electrode chamber was filled with excess of $\text{CuPF}_6(\text{MeCN})_4$ dissolved in 0.1 M TBAPF₆/MeCN solution (1 mL). The auxiliary electrode was made with a platinum wire wrapped with copper wire (diam. 0.25 mm, 99.999% trace metals basis from Sigma Aldrich). The whole apparatus was subjected to different potentials of -0.50 , $+0.10$, and $+0.42$ V (vs Ag/AgCl), respectively. After retaining the each potentials for 10 min, 1 mL of each solution was drawn out from the working cell corresponding to +4, +6, and +7 states of **mHe[2]C•nPF₆** respectively. Each of the three solutions was injected into a 2-mm path cuvette which sealed by Teflon caps and then was analyzed by using Vis/NIR spectroscopy. For **mHe[2]C•nPF₆**, the +4, +6, and +7 states were obtained using the same protocol under the potentials of -0.50 , $+0.10$, and $+0.50$ V, respectively. The +6 states (bisradical hexacationic states) of **mHo[2]C•nPF₆** and **mHe[2]C•nPF₆** were exposed to air for several days and the Vis/NIR spectra were recorded to test their air-stability.

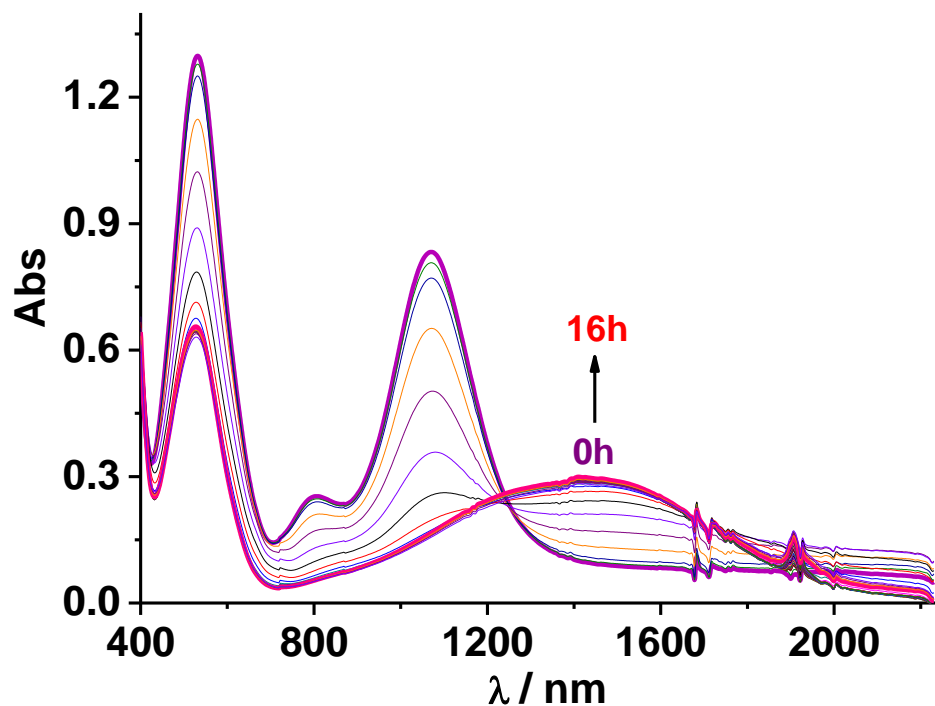


Figure S6. Time-dependent Vis/NIR absorption spectra in 30 min intervals (MeCN, optical length: 2 mm) of $m\text{Ho}[2]\text{C}^{4(\bullet\bullet)}$ upon exposing under ambient conditions for 16h.

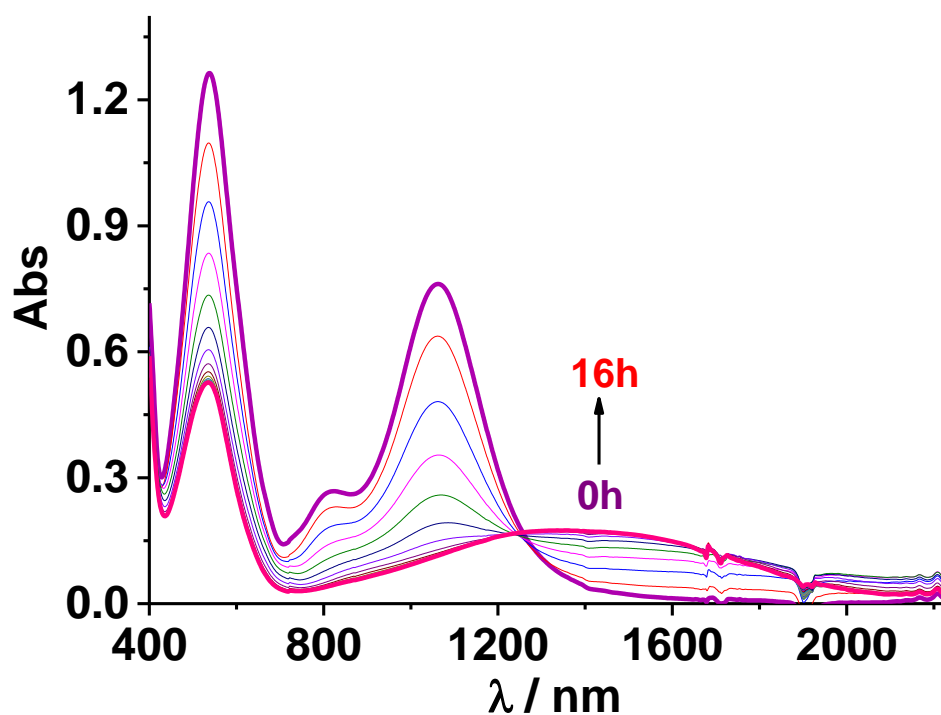


Figure S7. Time-dependent Vis/NIR absorption spectra in 30 min intervals (MeCN, optical length: 2 mm) of $m\text{Ho}[2]\text{C}^{4(\bullet\bullet)}$ upon exposing under ambient conditions for 16h.

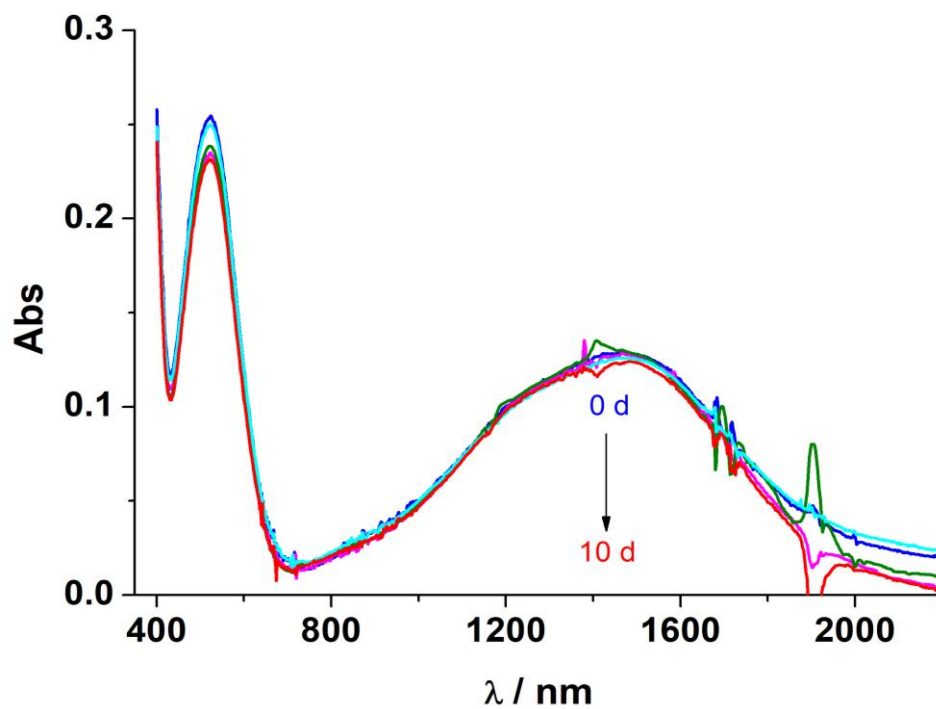


Figure S8. Time-dependent Vis/NIR absorption spectra (10 mM, MeCN, optical length: 2 mm) of $m\text{He}[2]\text{C}^{2+6+}$ upon exposing under ambient conditions.

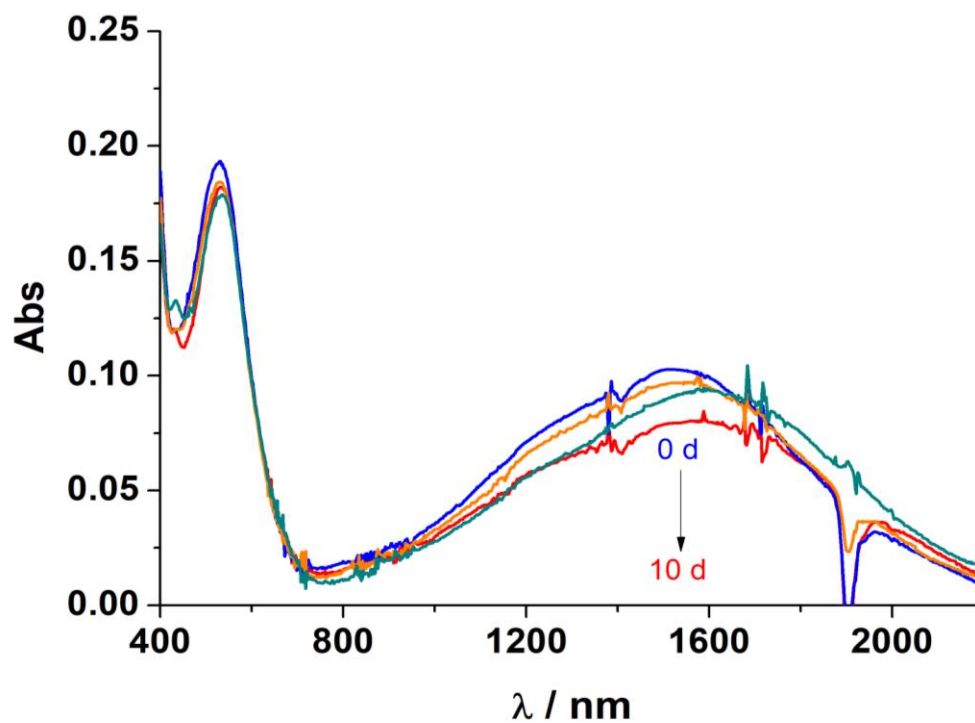


Figure S9. Time-dependent Vis/NIR absorption spectra (10 mM, MeCN, optical length: 2 mm) of $m\text{Ho}[2]\text{C}^{2+6+}$ upon exposing under ambient conditions.

Section E. Crystallographic Characterization

All crystallographic data are available free of charge from the Cambridge Crystallographic Data Centre (CDCC 1985179-1985180) via www.ccdc.cam.ac.uk/data_request/cif.

1) ***m*He[2]C•6PF₆**

a) Methods. Single crystals of ***m*He[2]C•6PF₆** were grown on the bench-top by slow vapor diffusion of ³Pr₂O into a 1.0 mM solution in MeCN over the course of a week. A suitable crystal was selected and mounted in inert oil and transferred to the cold gas stream of a Bruker Kappa Apex2 diffractometer. The crystal was kept at 100 K during data collection. Using Olex2^{S2}, the structure was solved with the XM^{S3} structure solution program using dual space and refined with the XL^{S4} refinement package using least squares minimization. The solid-state structure of ***m*He[2]C•6PF₆** is shown in Figure S8.

b) Crystal data. Triclinic, space group $P\bar{1}$ (no. 2), $a = 14.1120(2)$, $b = 15.2780(2)$, $c = 23.3050(3)$ Å, $\alpha = 84.5780(10)$, $\beta = 82.1550(10)$, $\gamma = 66.5170(10)^\circ$, $V = 4560.90(11)$ Å³, $Z = 2$, $T = 100.01(10)$ K, $\mu(\text{CuK}\alpha) = 2.200$ mm⁻¹, $D_{\text{calc}} = 1.481$ g/mm³, 58617 reflections measured ($3.83 \leq 2\theta \leq 146.334$), 17719 unique ($R_{\text{int}} = 0.0557$, $R_{\text{sigma}} = 0.0565$) which were used in all calculations. The final R_1 was 0.0960 ($I > 2\sigma(I)$) and wR_2 was 0.3126 (all data).

c) Refinement details. The enhanced rigid-bond restraint (SHELX keyword RIGU) was applied on the disordered PF₆⁻ anions. Distance restraints were also imposed on the disordered anions.

d) Solvent treatment details. The solvent masking procedure as implemented in Olex2^{S2} was used to remove the electronic contribution of solvent molecules from the refinement. As the exact solvent content is not known, only the atoms used in the refinement model are reported in the formula here.

2) ***m*Ho[2]C•6PF₆**

a) Methods. Single crystals of ***m*Ho[2]C•6PF₆** were grown on the bench-top by slow vapor diffusion of ³Pr₂O into a 1.0 mM solution in MeCN over the course of a week. A suitable single crystal was selected and mounted in inert oil and transferred to the cold gas stream of a Bruker APEX-II CCD diffractometer. The crystal was kept at 100 K during data collection. Using Olex2^{S2}, the structure was solved with the XM^{S3} structure solution program using dual space and refined with the XL^{S4} refinement package using least squares minimization.

b) *Crystal data.* Orthorhombic, space group Pna2₁ (no. 33), $a = 27.2161(4)$, $b = 20.3618(3)$, $c = 16.7417(3)$ Å, $V = 9277.7(3)$ Å³, $Z = 4$, $T = 100.01(10)$ K, $\mu(\text{CuK}\alpha) = 2.163$ mm⁻¹, $D_{\text{calc}} = 1.456$ g/mm³, 65212 reflections measured ($5.42 \leq 2\theta \leq 154.996$), 17763 unique ($R_{\text{int}} = 0.0527$, $R_{\text{sigma}} = 0.0496$) which were used in all calculations. The final R_1 was 0.0609 ($I > 2\sigma(I)$) and wR_2 was 0.1712 (all data).

c) *Refinement details.* Distance restraints were imposed on the disordered PF₆⁻ anions. The enhanced rigid-bond restraint (SHELX keyword RIGU) was applied to the disordered PF₆⁻ anions.

d) *Solvent treatment details.* The solvent masking procedure as implemented in Olex2 was used to remove the electronic contribution of solvent molecules from the refinement. As the exact solvent content is not known, only the atoms used in the refinement model are reported in the formula here. Total solvent accessible volume / cell = 3555.8 Å³ [32.0%] Total electron count / cell = 429.5

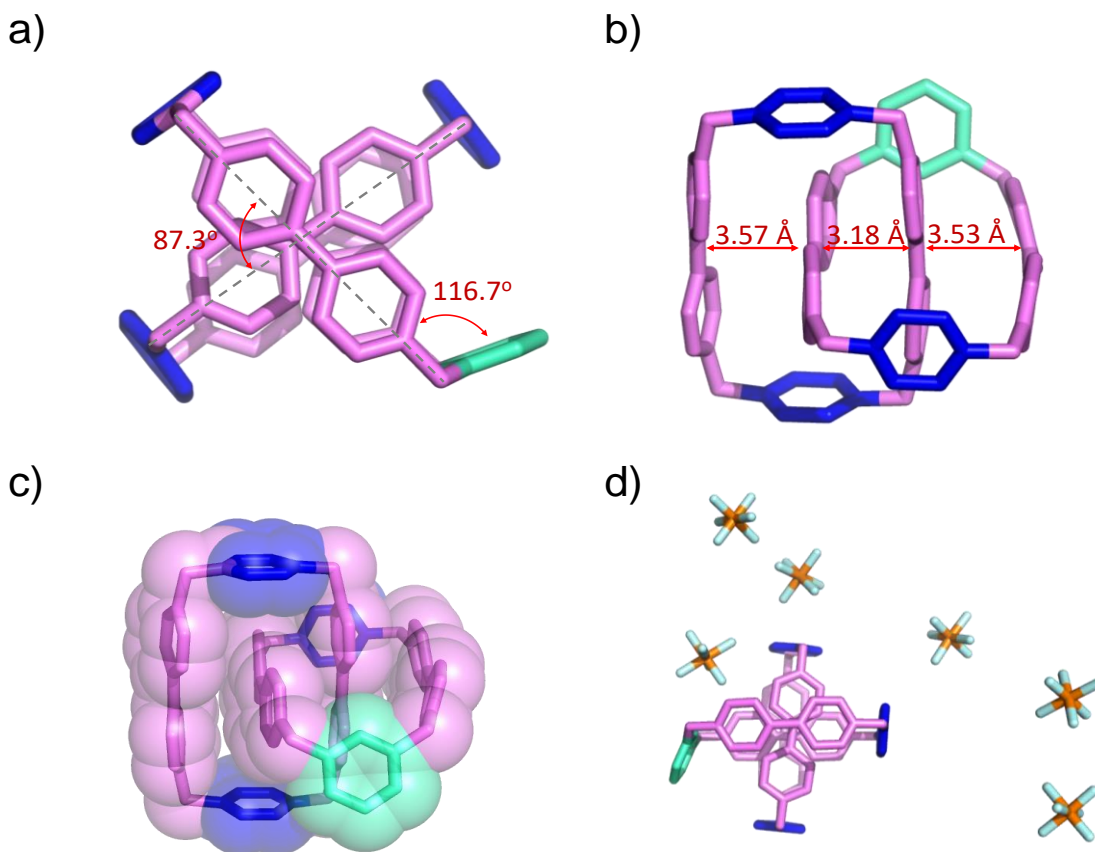


Figure S10. Tubular representation of the solid-state structure of **mHe[2]C²⁺⁶⁺**. a) A side-on view showing the dihedral angle between the BIPY units. b) A perspective view showing the distances between stacked units. c) Superimposed space-filling representation. d) A side-on view showing that there are six PF₆⁻ anions surrounding the catenane. Solvent molecules are omitted for the sake of clarity.

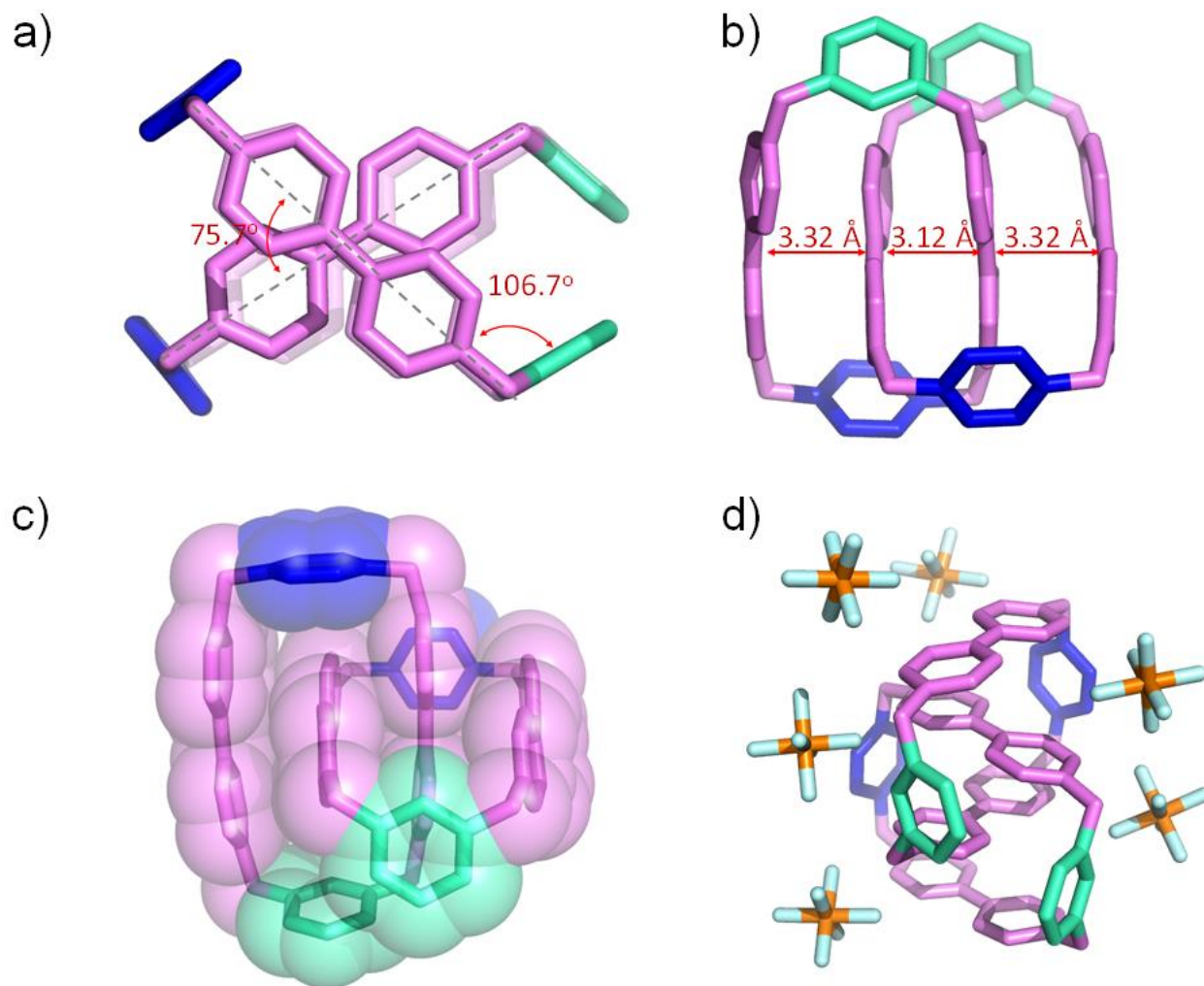


Figure S11. Solid-state structure of $mHo[2]C^{2+6+}$. a) A side-on view showing the dihedral angle between the BIPY units. b) A perspective view showing the distances between stacked units. c) Space-filling representation. d) A side-on view showing that there are six PF_6^- anions surrounding the catenane. Solvent molecules are omitted for the sake of clarity.

Section F. Summary of DFT Calculations

Method. Calculations were performed using density functional theory (DFT) with the M06 functional, as implemented^{S5} in Jaguar 7.6.110. Geometry optimizations were performed^{S6} using the 6-31G* basis set. Electronic energies (Table S1) were obtained^{S7} using the 6-311++G** basis set. Solvent corrections were based on single point self-consistent Poisson-Boltzmann continuum solvation calculations for MeCN ($\epsilon = 37.5$ and $R_0 = 2.179$ Å) using^{S8} the PBF module in Jaguar.

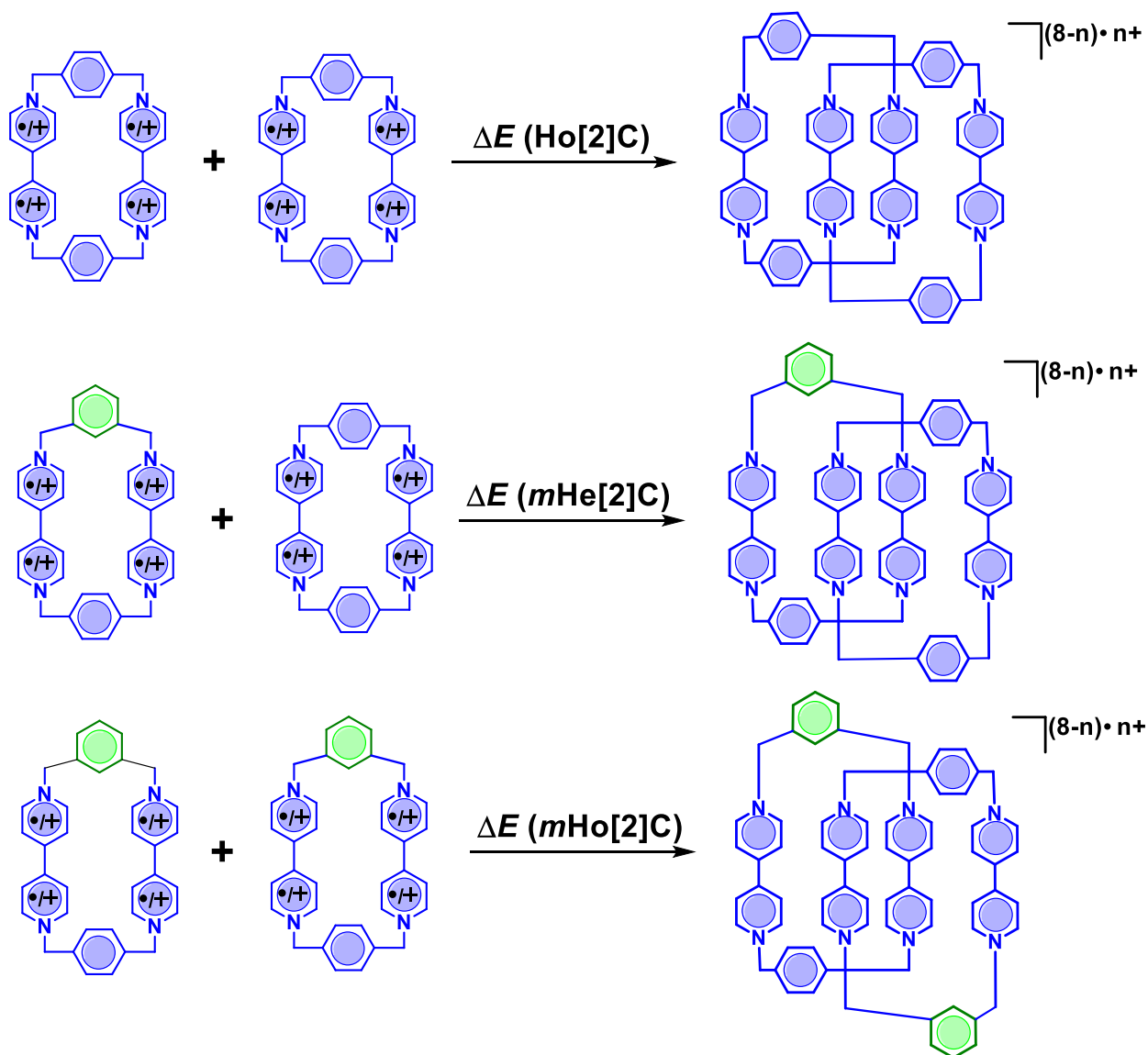


Table S1. Calculated Association Energies (ΔE) of [2]Catenanes

Charged State	ΔE (Ho[2]C) / (kcal mol ⁻¹)	ΔE (mHe[2]C) / (kcal mol ⁻¹)	ΔE (mHo[2]C) / (kcal mol ⁻¹)
0	-29.0	-25.5	-20.6
1+	-42.3	-40.5	-35.6
2+	-50.5	-48.7	-44.8
3+	-59.7	-58.2	-55.0
4+	-64.1	-60.0	-55.7
5+	-49.0	-41.6	-39.0
6+	-26.8	-14.6	-12.5
7+	-0.40	9.3	13.5
8+	40.2	55.6	58.9

Table S2. Calculated Association Energy Differences ($\Delta\Delta E$) Between Different Charged States

	$\Delta\Delta E$ (Ho[2]C) / (kcal mol ⁻¹)	$\Delta\Delta E$ (mHe[2]C) / (kcal mol ⁻¹)	$\Delta\Delta E$ (mHo[2]C) / (kcal mol ⁻¹)
8+ to 7+ ^a	-44.2	-46.3	-45.4
8+ to 6+ ^b	-67	-70.2	-71.4

^a $\Delta\Delta E = \Delta E_{7+} - \Delta E_{8+}$; ^b $\Delta\Delta E = \Delta E_{6+} - \Delta E_{8+}$

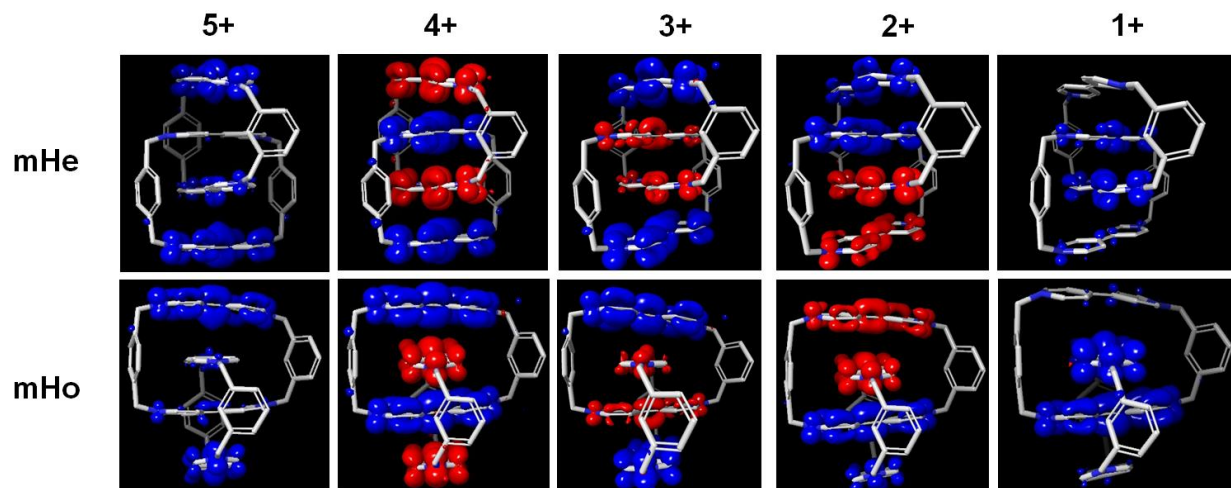


Figure S12. Spin-density distribution of two [2]catenane molecules with different positive charges.

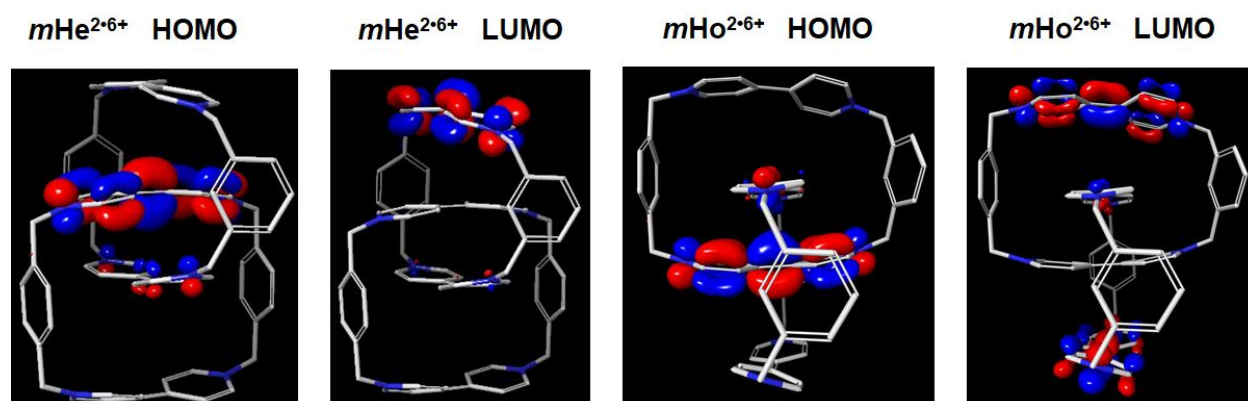


Figure S13. DFT calculated HOMOs and LUMOs for *mHe*[2]*C*²⁺⁶⁺ and *mHo*[2]*C*²⁺⁶⁺.

The cartesian coordinates and the single point energy calculated at M06/6-311++G** of the following species are provided: 1. CBPQTⁿ⁺, n=0-4, 2. mCBPQTⁿ⁺, n=0-4, 3. mHeⁿ⁺, n=0-8, 4. mHoⁿ⁺, n=0-8

CBPQT⁰ -1609.20446666897

N1	17.6313843280	15.4776828746	2.0281030373
C2	19.0941387182	15.4571017794	2.1350335872
C3	16.8852621550	16.0752410098	3.0399798231
C4	16.9910739717	14.4920890304	1.2819072520
C5	19.5971069606	14.4156882025	3.1005187291
H6	19.4123727267	16.4593259532	2.4454850187

H7	19.4938158939	15.2796974054	1.1295060899
H8	17.4162473883	16.8260592801	3.6179698095
C9	15.5828845335	15.7813134674	3.2564681170
C10	15.6894910820	14.1704999271	1.4623703435
H11	17.6060883952	14.0235678125	0.5182538553
C12	19.7465344721	14.7148231073	4.4587321884
C13	19.8535702939	13.1094742874	2.6705784020
H14	15.0773794646	16.3423375477	4.0362845739
C15	14.8641859060	14.7869596235	2.4836166723
H16	15.2754313647	13.4184895481	0.7974428668
C17	20.1322050435	13.7314678772	5.3645771227
H18	19.5700572053	15.7323783246	4.8070332689
H19	19.7612855335	12.8646443701	1.6124640893
C20	20.2389734627	12.1259322556	3.5763987379
C21	13.5298697009	14.4582346366	2.7016535564
C22	20.3774851780	12.4224999287	4.9363525741
H23	20.2553867118	13.9836646384	6.4178455309
H24	20.4455472040	11.1157039655	3.2230487033
C25	12.7102219157	15.0649522599	3.7326853830
C26	12.8098028327	13.4641264800	1.9293181154
C27	20.7076557850	11.3384397719	5.9292256608
H28	13.1161236339	15.8407241431	4.3743403321
C29	11.4224338250	14.7107465720	3.9454292936
C30	11.5191523999	13.1420430792	2.1742844050
H31	13.2943123836	12.9527837663	1.1030864056
N32	19.5159636347	10.6655485937	6.4567085071
H33	21.3392101896	10.5694889881	5.4684907319
H34	21.2574419691	11.7500289807	6.7839923615
N35	10.7647859372	13.7693445678	3.1605854495
H36	10.8147138010	15.1646107929	4.7231515706
H37	10.9828229072	12.4008730755	1.5889385553
C38	18.7505124381	11.3012713841	7.4307001936
C39	18.8649074685	9.7190970167	5.6713370846
C40	9.5718598174	13.1003380938	3.6888407793
C41	17.4592940550	10.9764110870	7.6702215216
H42	19.2778336652	12.0553210256	8.0092292805
H43	19.4815570707	9.2557660924	4.9056559416
C44	17.5750691395	9.3662415534	5.8750953404
H45	8.9438395693	13.8686666008	4.1543444321
H46	9.0191940083	12.6943447944	2.8337136642
C47	9.9008356292	12.0107724552	4.6758729521
C48	16.7471938255	9.9749646786	6.8991966615
H49	16.9654937319	11.5008432918	8.4833984341
H50	17.1765392553	8.5809213273	5.2397136213
C51	10.0494596401	12.3015860470	6.0356360884
C52	10.1373648471	10.7029640428	4.2410219095

C53	15.4132995332	9.6415805177	7.1115593755
H54	9.8494242962	13.3109924302	6.3942106076
C55	10.4357449298	11.3132736421	6.9351620994
C56	10.5233904363	9.7140449037	5.1406264493
H57	10.0064253304	10.4558935534	3.1876452634
C58	14.5864053665	10.2484483050	8.1374477730
C59	14.6964927746	8.6530278062	6.3288405745
H60	10.5365825456	11.5535373636	7.9933860415
C61	10.6832160381	10.0075614874	6.4988960892
H62	10.6927121931	8.6968807820	4.7873663654
C63	13.2874129957	9.9197639269	8.3194259382
H64	15.0022419416	10.9907356836	8.8127110181
H65	15.1985024820	8.1078359184	5.5341349811
C66	13.3947630449	8.3557453109	6.5429706742
C67	11.1861818205	8.9601420488	7.4576928014
N68	12.6492502584	8.9382012444	7.5658896490
H69	12.6747750398	10.3748728161	9.0934619318
H70	12.8622536433	7.6153801074	5.9516605124
H71	10.7873341430	9.1325049834	8.4643711446
H72	10.8662570492	7.9601795606	7.1415972743

CBPQT¹⁺ -1609.07633707740

N1	17.6217129315	15.4506277502	2.1520857850
C2	19.0913441366	15.5172329579	2.2199758682
C3	16.8583694370	16.0623701372	3.1239320656
C4	17.0101266925	14.5166869247	1.3416028563
C5	19.6389507837	14.4576694581	3.1404965414
H6	19.3570836234	16.5229219498	2.5630231708
H7	19.4731449718	15.3965587762	1.2003980721
H8	17.3773239535	16.7957625865	3.7342510998
C9	15.5393330287	15.7791442328	3.2865377543
C10	15.6942245997	14.2004014941	1.4709846274
H11	17.6458817720	14.0687412894	0.5836615578
C12	19.7746726802	14.7049765206	4.5109014507
C13	19.9311339224	13.1789649696	2.6549933175
H14	15.0125719987	16.3274568433	4.0607803832
C15	14.8628246117	14.7977646842	2.4813434881
H16	15.2923615283	13.4744520989	0.7719364617
C17	20.1672611609	13.6904407516	5.3776678193
H18	19.5756197504	15.7027523779	4.9013028550
H19	19.8556995956	12.9786049773	1.5864553109
C20	20.3215453765	12.1634290668	3.5224235186
C21	13.5107709864	14.4422393830	2.6769740650
C22	20.4314114456	12.4034330644	4.8959319973
H23	20.2745221001	13.9001837027	6.4417041989
H24	20.5487087626	11.1729204576	3.1287829934

C25	12.6781905160	15.0511102740	3.6792851396
C26	12.8443562217	13.4284335127	1.9038900895
C27	20.7274264517	11.2761141958	5.8503670824
H28	13.0512750853	15.8581408839	4.3013297562
C29	11.3959730058	14.6550643071	3.8918470968
C30	11.5593721471	13.0605231503	2.1540340026
H31	13.3516403454	12.9183005655	1.0917278969
N32	19.4861697792	10.6585439814	6.3445247636
H33	21.3176136893	10.4891739302	5.3682314761
H34	21.2858251521	11.6282337073	6.7246941163
N35	10.8046428126	13.6617609298	3.1400276976
H36	10.7625754493	15.1096141119	4.6479626178
H37	11.0513821166	12.2895589264	1.5821563966
C38	18.7971022322	11.2391184500	7.3902851745
C39	18.8217498296	9.7244997991	5.5742802198
C40	9.5616360046	13.0285803190	3.6119128682
C41	17.5108255109	10.9096968637	7.6760743301
H42	19.3597617037	11.9587106514	7.9781499925
H43	19.4022927742	9.2893067727	4.7659073197
C44	17.5367324816	9.3617624247	5.8271035756
H45	8.9255000377	13.8217114931	4.0197414685
H46	9.0553332617	12.6059675216	2.7375645297
C47	9.8512707784	11.9710274506	4.6450234935
C48	16.7699447040	9.9562554008	6.8917879540
H49	17.0594835704	11.3959407346	8.5349839525
H50	17.1066461819	8.6012195550	5.1834559148
C51	9.9899164292	12.3159065895	5.9940200476
C52	10.0799236845	10.6454568267	4.2622425691
C53	15.4168456157	9.6453055093	7.1348513380
H54	9.7883403568	13.3383670758	6.3127367417
C55	10.3776877978	11.3649278598	6.9321071694
C56	10.4637452331	9.6932830544	5.2014230988
H57	9.9516372131	10.3567258466	3.2193054428
C58	14.6349459104	10.2734988405	8.1689481874
C59	14.6821677173	8.6793370592	6.3602245748
H60	10.4801493765	11.6480843517	7.9793713433
C61	10.6323360726	10.0450696857	6.5450216260
H62	10.6308309274	8.6626771651	4.8888865836
C63	13.3145110936	10.0005122984	8.3415388147
H64	15.0785500864	10.9956975803	8.8466911437
H65	15.1680233543	8.1063946376	5.5769722629
C66	13.3635032996	8.4335179213	6.5713678888
C67	11.1769215936	9.0478473744	7.5342792318
N68	12.6482042966	9.0763535177	7.5617295567
H69	12.7159532865	10.4786796604	9.1116392005
H70	12.8048870507	7.7070184164	5.9883585195

H71	10.8263182462	9.2583334032	8.5503040705
H72	10.8739513146	8.0265477123	7.2778375109

CBPQT²⁺ -1608.95447310689

N1	17.5984053016	15.3962406138	2.1499768044
C2	19.0760684180	15.4694690909	2.1910591608
C3	16.8527625061	16.0461294201	3.0978930150
C4	16.9722333639	14.5120107269	1.3103199339
C5	19.6298040616	14.4252976122	3.1300997889
H6	19.3429381077	16.4824860443	2.5082019432
H7	19.4382386040	15.3273904806	1.1681070738
H8	17.3892063098	16.7567025521	3.7195007000
C9	15.5158452714	15.8097908865	3.2410180025
C10	15.6371364971	14.2433361848	1.4187908094
H11	17.6011821815	14.0466619614	0.5574024206
C12	19.8020185118	14.7080752227	4.4891888493
C13	19.9027546168	13.1330139647	2.6700063203
H14	14.9995816856	16.3707438609	4.0125877612
C15	14.8316629545	14.8559272729	2.4272715805
H16	15.2191202208	13.5382522017	0.7084500466
C17	20.2019416725	13.7104401983	5.3746492507
H18	19.6231573014	15.7168717616	4.8597267913
H19	19.8033096257	12.9039311336	1.6096971459
C20	20.3013798808	12.1354449288	3.5554183880
C21	13.4553779424	14.5138901446	2.6326303813
C22	20.4370322186	12.4086394477	4.9202980955
H23	20.3322814370	13.9473148354	6.4300174594
H24	20.5098838861	11.1341318041	3.1805222171
C25	12.6550774699	15.1180298270	3.6498234584
C26	12.7864718542	13.5151451623	1.8616160488
C27	20.7392804937	11.2975751976	5.8964632499
H28	13.0360353882	15.9250107195	4.2663958100
C29	11.3792837047	14.7011168567	3.8988121249
C30	11.5088499132	13.1275588470	2.1469352865
H31	13.2759349771	13.0177933061	1.0310215122
N32	19.4809247743	10.6849645950	6.3761677314
H33	21.3356216943	10.5033394761	5.4371670445
H34	21.2791236491	11.6635377530	6.7752966380
N35	10.7986270736	13.6957966822	3.1714513589
H36	10.7631329304	15.1416005784	4.6767649363
H37	10.9932145130	12.3574726050	1.5813958093
C38	18.7996936072	11.2505638295	7.4216642681
C39	18.8706374783	9.6985144724	5.6467231958
C40	9.5417834849	13.0723633362	3.6405584407
C41	17.5214611108	10.8802482378	7.7247240659
H42	19.3388720697	12.0031093098	7.9890225988

H43	19.4643070360	9.2620142565	4.8492466454
C44	17.5940345431	9.2947879984	5.9160689788
H45	8.9227781292	13.8673592675	4.0675602233
H46	9.0259018184	12.6738838691	2.7616202279
C47	9.8443036107	11.9934553092	4.6520433380
C48	16.8235137625	9.9005751192	6.9552637824
H49	17.0564062321	11.3715655071	8.5726818701
H50	17.1882726857	8.5039729420	5.2946318373
C51	9.9644121248	12.3071993740	6.0096642696
C52	10.0956815071	10.6815608813	4.2376076237
C53	15.4465751099	9.5794978878	7.1842063637
H54	9.7440243503	13.3171602054	6.3532406001
C55	10.3631751477	11.3392644614	6.9275006264
C56	10.4928214654	9.7131623174	5.1556923198
H57	9.9792419407	10.4140617628	3.1880262095
C58	14.6590096370	10.2305726113	8.1825802056
C59	14.7441501592	8.6102455035	6.4055650010
H60	10.4518636062	11.5997700558	7.9815122836
C61	10.6490210447	10.0362752241	6.5077834182
H62	10.6823890534	8.6953852294	4.8166072104
C63	13.3219232808	9.9819094750	8.3109654840
H64	15.0910637699	10.9551689302	8.8641704616
H65	15.2478143632	8.0184755909	5.6487729400
C66	13.4070402742	8.3913798299	6.5709421947
C67	11.1997826519	9.0209984380	7.4797914047
N68	12.6782146663	9.0788076528	7.5055221681
H69	12.7049554772	10.4793494207	9.0532238789
H70	12.8572929556	7.6656259003	5.9792456094
H71	10.8481252542	9.2026455316	8.4999859411
H72	10.9200310184	8.0004362720	7.2006287147

CBPQT³⁺ -1608.79255604337

N1	17.5955995357	15.4427612970	2.1328608363
C2	19.0863752286	15.5020546083	2.1807716716
C3	16.8716970161	16.0362609602	3.1199067062
C4	16.9662902198	14.6658420929	1.2104605520
C5	19.6050192367	14.4423553801	3.1238667065
H6	19.3569355565	16.5120189349	2.5035563779
H7	19.4477373345	15.3616287100	1.1574699461
H8	17.4212421245	16.6734698267	3.8066366051
C9	15.5221975443	15.8140660361	3.2415112758
C10	15.6164528217	14.4141781402	1.2932935468
H11	17.5882211807	14.2566543256	0.4193187593
C12	19.8160527993	14.7299659128	4.4769685910
C13	19.8149130792	13.1347921323	2.6705818361
H14	15.0159196855	16.2961619429	4.0711480480

C15	14.8443382304	14.9477889038	2.3521252465
H16	15.1816381794	13.7940523166	0.5158128291
C17	20.1988691198	13.7252217258	5.3635557355
H18	19.6869215403	15.7482295710	4.8423551083
H19	19.6835886803	12.8984080041	1.6152870244
C20	20.1983580141	12.1315546982	3.5559035612
C21	13.4485371111	14.5800117741	2.5632665202
C22	20.3794928596	12.4120632626	4.9154963002
H23	20.3647847120	13.9687315265	6.4126030562
H24	20.3655465016	11.1216164749	3.1829252616
C25	12.6367014237	15.2239330067	3.5271044860
C26	12.8486133501	13.5098176781	1.8601933474
C27	20.6946338103	11.3006050869	5.8882181438
H28	12.9741282650	16.0968034185	4.0770087889
C29	11.3722011717	14.7630510164	3.8050615058
C30	11.5816626562	13.0813496294	2.1734524469
H31	13.3772075848	12.9650936279	1.0848949385
N32	19.4311983863	10.6798401004	6.3758697686
H33	21.2852441174	10.5037350963	5.4257451773
H34	21.2351509062	11.6621002779	6.7687343306
N35	10.8591629927	13.6827348018	3.1566493979
H36	10.7322318726	15.2298192719	4.5482311113
H37	11.1087601633	12.2437575111	1.6688824982
C38	18.7769222028	11.2206352983	7.4420720833
C39	18.8385714209	9.6818076228	5.6612536359
C40	9.5945979692	13.0520183105	3.6355980314
C41	17.5076624051	10.8207652626	7.7746869367
H42	19.3131427220	11.9817394547	8.0017279194
H43	19.4224503116	9.2604037469	4.8479591092
C44	17.5702456458	9.2487159094	5.9577711823
H45	8.9735355831	13.8519933388	4.0498119981
H46	9.0865226075	12.6451289378	2.7561919336
C47	9.9097881023	11.9826857978	4.6542653117
C48	16.8239606889	9.8387230463	7.0112148205
H49	17.0539596259	11.2997412540	8.6362217345
H50	17.1646720193	8.4576746867	5.3360087556
C51	10.0737431484	12.3136686885	6.0045992598
C52	10.1037952901	10.6557208215	4.2555484254
C53	15.4314778744	9.5011683864	7.2535972902
H54	9.8993346610	13.3357562336	6.3387111636
C55	10.4489447858	11.3442998242	6.9305549021
C56	10.4802236713	9.6858205828	5.1820298407
H57	9.9526041982	10.3745176436	3.2140022700
C58	14.6564106579	10.1576645397	8.2450302716
C59	14.7423946358	8.5344462462	6.4760473325
H60	10.5640002866	11.6184176043	7.9788181288
C61	10.6705406378	10.0223930063	6.5266711711
H62	10.6217217601	8.6560487749	4.8552426250

C63	13.3098865809	9.9233240098	8.3625232741
H64	15.0889580224	10.8819727665	8.9272649521
H65	15.2466878826	7.9323604826	5.7273511881
C66	13.3943768829	8.3318063123	6.6294557369
C67	11.1841341745	8.9970588725	7.5092563704
N68	12.6725872052	9.0404622791	7.5428998614
H69	12.6928871305	10.4289741849	9.0996850353
H70	12.8421827594	7.6112348117	6.0331880203
H71	10.8338143137	9.1873521721	8.5285429627
H72	10.8972142566	7.9780142090	7.2313513526

CBPQT⁴⁺ -1608.63717568326

N1	17.5292627350	15.5936175791	2.2621533317
C2	19.0268675604	15.6441961902	2.3768987787
C3	16.7795765376	16.0433246384	3.2955237778
C4	16.9466092359	14.9902388427	1.1999351061
C5	19.5108102873	14.4897477791	3.2282761678
H6	19.2773043392	16.6150479297	2.8140809242
H7	19.4238537053	15.6103768321	1.3583048586
H8	17.3044310951	16.5586807479	4.0951101641
C9	15.4184455650	15.8164982174	3.3284600227
C10	15.5860643921	14.7399840208	1.1863840484
H11	17.6009605255	14.6999123335	0.3825507698
C12	19.7384671881	14.6603441513	4.5985487144
C13	19.7038475420	13.2229407514	2.6648000701
H14	14.8693554671	16.1510320344	4.2038336062
C15	14.7961208726	15.1060787979	2.2882924585
H16	15.1687037549	14.2505091492	0.3112835040
C17	20.1268486615	13.5818936513	5.3928244196
H18	19.6236354642	15.6440390034	5.0516880618
H19	19.5622233709	13.0739505659	1.5953437088
C20	20.0926317544	12.1452857870	3.4579411689
C21	13.3882290920	14.6693459716	2.4262111841
C22	20.2974256380	12.3101067859	4.8334873156
H23	20.3086215376	13.7398969943	6.4550953046
H24	20.2520086206	11.1716811990	2.9961524440
C25	12.4680835631	15.3601482930	3.2311940054
C26	12.9611481979	13.4696967131	1.8332708121
C27	20.6630632799	11.1263483401	5.7027007089
H28	12.6959686161	16.3270943543	3.6721960759
C29	11.2282501390	14.8061284437	3.4938398270
C30	11.7129285009	12.9575494085	2.1248640921
H31	13.6094830325	12.8878145467	1.1846367395
N32	19.4176116820	10.4973763610	6.2611087609
H33	21.1850283360	10.3451702687	5.1419571133
H34	21.2840069790	11.4104152540	6.5574448654
N35	10.8833827995	13.6037694678	2.9770417736
H36	10.4954382410	15.2926604989	4.1315422007

H37	11.3580074907	12.0169620210	1.7128008961
C38	18.9549006894	10.8766732495	7.4751885779
C39	18.7020957844	9.6487892699	5.4862421791
C40	9.6399396522	12.9058885801	3.4511724146
C41	17.7062793119	10.4759380325	7.9126696723
H42	19.6021790862	11.5185913438	8.0666546892
H43	19.1513343744	9.3482502150	4.5436846631
C44	17.4480134693	9.2238236403	5.8781753638
H45	8.9483590873	13.6838616168	3.7867448234
H46	9.2056468164	12.4101661239	2.5781829911
C47	9.9910372827	11.9268895487	4.5502907186
C48	16.8972318682	9.6763830396	7.0889480450
H49	17.3825249167	10.8082680266	8.8954664916
H50	16.8934794122	8.5875423908	5.1953800720
C51	10.0941578116	12.3555100838	5.8787394742
C52	10.2524322694	10.5845928383	4.2519769963
C53	15.4781844633	9.4076645177	7.4109028640
H54	9.8669569697	13.3884297515	6.1382556299
C55	10.4714678440	11.4664142941	6.8835741603
C56	10.6313797657	9.6953511138	5.2565496582
H57	10.1486389513	10.2235564607	3.2296244224
C58	14.7487069297	10.3095132457	8.2038630957
C59	14.7839242601	8.3194793661	6.8577723227
H60	10.5310056212	11.8170752830	7.9130942955
C61	10.7555206043	10.1288556350	6.5816258498
H62	10.8209049205	8.6530629375	5.0035434560
C63	13.3809666380	10.1687384645	8.3323550519
H64	15.2164971852	11.1646515100	8.6824543195
H65	15.2852257237	7.5382898522	6.2928061375
C66	13.4136591744	8.2226239838	7.0137058055
C67	11.2260312020	9.1801813099	7.6630828930
N68	12.7279686946	9.1623954993	7.7054814601
H69	12.7747069638	10.8625863286	8.9082629064
H70	12.8325718357	7.4144640518	6.5779532233
H71	10.8864135988	9.4841702441	8.6573264323
H72	10.9028904760	8.1498185557	7.4880018736

mCBPQT⁰ -1609.20177349681

N1	5.5231136425	2.1383383501	10.7457405514
C2	6.8527546288	2.5129640653	11.2448339761
C3	4.7871650815	1.1757288491	11.4362524606
C4	4.7858356295	3.0994292909	10.0523967260
C5	6.7927994847	3.5336456973	12.3500617524
H6	7.4278821839	2.9011158992	10.3956291706
H7	7.3417840957	1.5920737084	11.5820702116
H8	5.3829305389	0.4546077535	11.9900707840
C9	3.4371732317	1.1100109614	11.3832597382
C10	3.4364525393	3.0775192455	9.9848651681

H11	5.3817254128	3.8509324611	9.5419577479
C12	6.5555585648	3.1432612086	13.6727662001
C13	6.8759467940	4.8987828058	12.0611655266
H14	2.9656738427	0.2881174368	11.9142538508
C15	2.6328459700	2.0763628808	10.6595181795
H16	2.9619308633	3.8450237733	9.3807304386
C17	6.3986765253	4.0925296259	14.6760778777
H18	6.4991698961	2.0829567820	13.9166363408
H19	7.0766056340	5.2190864863	11.0388001201
C20	6.7163311035	5.8494145629	13.0655758782
C21	1.2425060988	2.0531268478	10.6197788012
C22	6.4711556663	5.4597821328	14.3850822717
H23	6.2198234625	3.7714290958	15.7016227320
H24	6.7900653937	6.9100398769	12.8252630949
C25	0.4380695171	1.0250226699	11.2521337417
C26	0.4403996545	3.0656225143	9.9586063323
C27	6.1955644034	6.4878594492	15.4500539344
H28	0.9099587504	0.2019971919	11.7802117499
C29	-0.9142009627	1.0277837416	11.2119903034
C30	-0.9126957724	3.0370785593	9.9550879484
H31	0.9116828288	3.9022299981	9.4523109719
N32	4.7606702198	6.7142115207	15.6681309859
H33	6.6451556267	7.4505257542	15.1790041275
H34	6.6223631470	6.1829478639	16.4120001958
N35	-1.6342334417	2.0128586070	10.5487679950
H36	-1.5139711420	0.2552646878	11.6847524834
H37	-1.5128515254	3.8024022441	9.4710914637
C38	4.0495349355	5.8114502209	16.4589704153
C39	4.0355408966	7.3603466800	14.6658828735
C40	-3.0831264369	2.0794378428	10.6937556428
C41	2.7159820405	5.6225400275	16.3350111141
H42	4.6413249159	5.3017781684	17.2150897555
H43	4.6177299789	8.0362530530	14.0456441573
C44	2.7041640319	7.1956711700	14.5043914003
H45	-3.5131354972	1.1207808294	10.3720245936
H46	-3.4404796416	2.8436378219	9.9951499006
C47	-3.5337010189	2.3820572459	12.1027692661
C48	1.9188729498	6.2953565781	15.3270543774
H49	2.2506747093	4.9377714782	17.0380518494
H50	2.2278985621	7.7830246633	13.7251632057
C51	-4.0523519276	1.3588126386	12.9032855171
C52	-3.4121252770	3.6660413546	12.6392397857
C53	0.5515506265	6.0986421655	15.1617824740
H54	-4.1566254561	0.3562737238	12.4885530458
C55	-4.4432670406	1.6164693984	14.2146598292
C56	-3.8063521569	3.9396111490	13.9514120744
H57	-3.0125059036	4.4702433402	12.0195729704
C58	-0.2402280752	5.2139350159	15.9955341264

C59	-0.2323840799	6.7426777757	14.1244318298
H60	-4.8471437428	0.8153347183	14.8295427390
C61	-4.3206514495	2.9020899734	14.7356748905
C62	-3.6574258006	5.3243524602	14.5352955141
C63	-1.5682192010	5.0319498693	15.8119808788
H64	0.2205669862	4.6636471868	16.8102557129
H65	0.2350265645	7.4219470533	13.4184814848
C66	-1.5592110747	6.5253552331	13.9713416269
H67	-4.6332068965	3.1095400335	15.7589784666
N68	-2.2772967640	5.6958143918	14.8191988066
H69	-4.2365955163	5.3933366111	15.4660369343
H70	-4.0567038908	6.0801395365	13.8505654854
H71	-2.1586178763	4.3676160321	16.4366733695
H72	-2.1435763997	7.0018063197	13.1892889087

mCBPQT¹⁺ -1609.07574833630

N1	5.4719889117	2.2380898452	10.8354375860
C2	6.8562105078	2.5533710377	11.2274738486
C3	4.7700228467	1.2520125855	11.4987885287
C4	4.7511536399	3.1589657939	10.1002436641
C5	6.8703971747	3.5628737558	12.3442219018
H6	7.3737060007	2.9335173606	10.3393238503
H7	7.3342887403	1.6127697944	11.5214094539
H8	5.3747658666	0.5479109898	12.0634248409
C9	3.4154806447	1.1581935375	11.4276188921
C10	3.3968640747	3.1094783731	10.0111048614
H11	5.3421068794	3.9113000258	9.5861505912
C12	6.7074939392	3.1545753304	13.6731921331
C13	6.9150956279	4.9316338549	12.0612635579
H14	2.9527652573	0.3333956624	11.9606121236
C15	2.6207209534	2.1084989411	10.6946564583
H16	2.9178569101	3.8554342322	9.3852198586
C17	6.5552576440	4.0922297741	14.6878180733
H18	6.6947562563	2.0915162709	13.9120794814
H19	7.0674135720	5.2646458379	11.0347067289
C20	6.7612780391	5.8702585172	13.0771779598
C21	1.2099451763	2.0707086133	10.6537248776
C22	6.5604103452	5.4616438664	14.3990948208
H23	6.4243465085	3.7589712214	15.7166876296
H24	6.7929021666	6.9336222060	12.8411721002
C25	0.4326561844	1.0388619834	11.2888141627
C26	0.4164154199	3.0675081006	9.9833219262
C27	6.2183451187	6.4678038534	15.4657157139
H28	0.9133427033	0.2200941074	11.8149121681
C29	-0.9254864947	1.0322815758	11.2523302821
C30	-0.9429129391	3.0266083666	9.9806569960
H31	0.8807661285	3.9016398363	9.4673908902
N32	4.7576425268	6.6047560124	15.5991619348

H33	6.6241782698	7.4564342468	15.2249115826
H34	6.6084597899	6.1715365634	16.4449831186
N35	-1.6415136093	2.0130003500	10.5973899542
H36	-1.5185166846	0.2553148324	11.7259913457
H37	-1.5499788030	3.7794208122	9.4863352298
C38	4.0523275310	5.7418753755	16.4147262870
C39	4.0501557294	7.2991506798	14.6364917257
C40	-3.1029710599	2.0433039589	10.7023437682
C41	2.7077189550	5.5821277606	16.3056084858
H42	4.6427387592	5.2181164000	17.1607757572
H43	4.6384193099	7.9721501859	14.0200761891
C44	2.7078432230	7.1627830686	14.4888180820
H45	-3.4900621680	1.0654869489	10.3897991372
H46	-3.4607145485	2.7831303945	9.9784292212
C47	-3.5758594047	2.3658590402	12.0998970936
C48	1.9324124737	6.2656541942	15.3044198193
H49	2.2364112164	4.9045764556	17.0101302944
H50	2.2336012741	7.7714084412	13.7261650370
C51	-4.1301247571	1.3620754118	12.9004570309
C52	-3.4380984332	3.6540375573	12.6232633495
C53	0.5474289939	6.0715281249	15.1306335108
H54	-4.2458399817	0.3565947110	12.4962844769
C55	-4.5383927578	1.6427990464	14.2020914350
C56	-3.8386944163	3.9457684804	13.9296504112
H57	-3.0168523589	4.4444018680	11.9999773884
C58	-0.2363233694	5.1983022292	15.9642308679
C59	-0.2146444045	6.7186029788	14.0951341554
H60	-4.9705200922	0.8574419199	14.8177871310
C61	-4.3891219060	2.9287790758	14.7154927854
C62	-3.6585183482	5.3313021524	14.5040368910
C63	-1.5675109798	5.0132254516	15.7693077002
H64	0.2177767113	4.6574392462	16.7881101673
H65	0.2571471431	7.4007221760	13.3958131571
C66	-1.5460633366	6.5003679422	13.9314479368
H67	-4.7068902373	3.1506749954	15.7337961351
N68	-2.2546298419	5.6616050477	14.7633839232
H69	-4.2115130696	5.4215413938	15.4466046994
H70	-4.0463699747	6.0965501467	13.8242283428
H71	-2.1630793475	4.3562036041	16.3961045110
H72	-2.1249756783	6.9813158225	13.1486830065

mCBPQT²⁺ -1608.95461539456

N1	5.4585192627	2.2211917640	10.8668766118
C2	6.8587895375	2.5225932843	11.2452855476
C3	4.7616675452	1.2379029976	11.5187236235
C4	4.7710020447	3.0987018741	10.0687494937
C5	6.8709055629	3.5488033610	12.3511294095

H6	7.3704612940	2.8843727242	10.3476197294
H7	7.3248039667	1.5803185938	11.5496632385
H8	5.3539173842	0.5533667741	12.1187992466
C9	3.4047199922	1.1305454754	11.4079902284
C10	3.4147229918	3.0338421505	9.9362758242
H11	5.3722559659	3.8379914769	9.5485038634
C12	6.7399230386	3.1530664112	13.6866172603
C13	6.8913521985	4.9137948802	12.0500826085
H14	2.9304379406	0.3197400219	11.9511128458
C15	2.6410671852	2.0588326222	10.6366688309
H16	2.9503251377	3.7558371265	9.2732220284
C17	6.5842261594	4.1011642594	14.6926817368
H18	6.7507563955	2.0937147712	13.9406265917
H19	7.0241631113	5.2391045796	11.0186657386
C20	6.7327067556	5.8628447919	13.0570179064
C21	1.2095433963	2.0301501352	10.5880633787
C22	6.5525741589	5.4654148952	14.3848146227
H23	6.4757473082	3.7764575830	15.7268955717
H24	6.7402499305	6.9229521280	12.8055214452
C25	0.4378192511	1.0158088981	11.2332880644
C26	0.4418752311	3.0306524831	9.9179665214
C27	6.2033243274	6.4794357387	15.4455237251
H28	0.9099815360	0.1885798507	11.7532595412
C29	-0.9264342124	1.0403909499	11.2228217229
C30	-0.9242776458	3.0191974984	9.9384715638
H31	0.9158416263	3.8489200288	9.3866983393
N32	4.7310250793	6.5834421278	15.5656490434
H33	6.5848778691	7.4753107228	15.1988583481
H34	6.5898622358	6.1981371938	16.4293833067
N35	-1.6214969472	2.0370400177	10.5874913044
H36	-1.5267571136	0.2774540708	11.7096134331
H37	-1.5233221456	3.7774556034	9.4429485385
C38	4.0456468949	5.7417509566	16.4017951996
C39	4.0269281641	7.3231965084	14.6516358537
C40	-3.0942387099	2.0825946317	10.6912531704
C41	2.6886229187	5.6084275189	16.3263792240
H42	4.6457950753	5.1983576409	17.1256204089
H43	4.6131097154	7.9957034835	14.0330579941
C44	2.6713571603	7.2186066853	14.5386349430
H45	-3.4820844725	1.1137552029	10.3571460387
H46	-3.4392191483	2.8402089058	9.9806348696
C47	-3.5501000000	2.3836953806	12.0985074959
C48	1.9202574494	6.3166328761	15.3524822014
H49	2.2221601156	4.9271023339	17.0302938870
H50	2.1899852463	7.8498430977	13.7995873189
C51	-4.0942600886	1.3661304324	12.8893311957
C52	-3.4209087180	3.6679273742	12.6358964787
C53	0.5104442870	6.1219515771	15.1877719251

H54	-4.2065908342	0.3648090632	12.4744304825
C55	-4.5000633769	1.6296655604	14.1954966063
C56	-3.8224261633	3.9414598975	13.9469263552
H57	-3.0141282575	4.4702629604	12.0180670671
C58	-0.2476973495	5.2374033746	16.0146991393
C59	-0.2408697840	6.7755239046	14.1642535241
H60	-4.9241787960	0.8340415762	14.8032258086
C61	-4.3614811724	2.9111358289	14.7234062787
C62	-3.6679316190	5.3249636359	14.5309482169
C63	-1.5791849054	5.0262675627	15.8029153830
H64	0.2090938740	4.7006293794	16.8396767432
H65	0.2233662400	7.4769720990	13.4795526587
C66	-1.5736704284	6.5333624428	13.9876374308
H67	-4.6811528914	3.1181648735	15.7441183645
N68	-2.2546077306	5.6612895315	14.7925027981
H69	-4.2113059344	5.4088702131	15.4782677166
H70	-4.0573197192	6.0949703660	13.8578732959
H71	-2.1678938037	4.3542184658	16.4202385642
H72	-2.1582270170	7.0180265560	13.2112697847

mCBPQT³⁺ -1608.79214610189

N1	5.4193463198	2.2430381236	10.8079835174
C2	6.8210678650	2.5817693109	11.1906113537
C3	4.7580448162	1.2454947754	11.4566006715
C4	4.7372450097	3.0565071034	9.9551893489
C5	6.7968432033	3.5746048591	12.3281197517
H6	7.3102808716	2.9837020557	10.2984478349
H7	7.3162715346	1.6459369453	11.4651535366
H8	5.3585815673	0.6024903325	12.0934041400
C9	3.4020749436	1.0813950157	11.3131063417
C10	3.3811923515	2.9320162470	9.7848855351
H11	5.3241818586	3.8024042766	9.4276205294
C12	6.7523871120	3.1335535191	13.6550492427
C13	6.7241555656	4.9478077471	12.0683409506
H14	2.9431388687	0.2744597429	11.8742666678
C15	2.6424103415	1.9595139719	10.5025117151
H16	2.9094911463	3.6114322193	9.0828981870
C17	6.5998954645	4.0433882789	14.6984273544
H18	6.8373639534	2.0705863369	13.8769010509
H19	6.7897336526	5.3115145756	11.0436668308
C20	6.5709740211	5.8575068758	13.1110385648
C21	1.1893344168	1.9030825921	10.4527337675
C22	6.4873862605	5.4132909704	14.4357824198
H23	6.5677835954	3.6830835978	15.7262202252
H24	6.5165414781	6.9232426469	12.8906203966
C25	0.4510177063	0.8645109924	11.0731388019
C26	0.4232341777	2.9154017387	9.8265269449
C27	6.1786340889	6.3851100987	15.5493986382

H28	0.9350776407	0.0148794495	11.5432848396
C29	-0.9201360545	0.8941062264	11.1036407581
C30	-0.9492232137	2.9058750676	9.8842778890
H31	0.8860862208	3.7466841614	9.3058820758
N32	4.6988349210	6.5226739503	15.6758307769
H33	6.5798299868	7.3848164374	15.3551660052
H34	6.5558148258	6.0422550807	16.5179281384
N35	-1.6186936263	1.9164943398	10.5338970472
H36	-1.5074860756	0.1135622023	11.5778766457
H37	-1.5585176320	3.6776134698	9.4229834960
C38	3.9988663320	5.6315495520	16.4308588680
C39	4.0326754299	7.4104213000	14.8865371738
C40	-3.0951423079	1.9863402242	10.7093921461
C41	2.6281580676	5.5682954455	16.3643988700
H42	4.5829470449	4.9726799640	17.0669815490
H43	4.6420916963	8.1309630897	14.3487951715
C44	2.6637504849	7.3798339404	14.7827771529
H45	-3.4978890564	1.0046301953	10.4407881259
H46	-3.4665766388	2.7121530161	9.9799939131
C47	-3.4691874099	2.3534969607	12.1273457683
C48	1.9041028445	6.4150525694	15.4901582854
H49	2.1362052624	4.8147473005	16.9712910569
H50	2.1963575702	8.1257245879	14.1469921083
C51	-3.8904755468	1.3530926644	13.0093420430
C52	-3.3948331526	3.6758971465	12.5803319406
C53	0.4699560992	6.2609736419	15.2859568362
H54	-3.9659205606	0.3236378950	12.6611703567
C55	-4.2324728282	1.6683996199	14.3219014417
C56	-3.7322997069	4.0010256586	13.8994540210
H57	-3.0928141637	4.4662730784	11.8912301099
C58	-0.3348882917	5.4684714597	16.1428514649
C59	-0.1895549700	6.8509009362	14.1805427450
H60	-4.5673934347	0.8864518240	14.9986784489
C61	-4.1524448041	2.9857123488	14.7658172520
C62	-3.6432056803	5.4229225066	14.4034560150
C63	-1.6602406523	5.2530554587	15.8598514388
H64	0.0591860697	5.0192236552	17.0496507339
H65	0.3360384358	7.4828548245	13.4718014154
C66	-1.5183628955	6.6021139531	13.9345118771
H67	-4.4339373502	3.2316608450	15.7894122942
N68	-2.2445353476	5.7944568484	14.7532229622
H69	-4.2463733588	5.5589304246	15.3073596926
H70	-3.9847508638	6.1486067596	13.6588999982
H71	-2.2992600185	4.6509059806	16.4982772326
H72	-2.0449473344	7.0267929521	13.0847414153

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N1	5.3793763640	2.1397247619	10.8065715315
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C4	4.7909941486	2.7771662558	9.7679736581
C5	6.7058229372	3.5223500957	12.3452393124
H6	7.2753947790	2.9030422165	10.3333910174
H7	7.2748982012	1.5846318269	11.5255614911
H8	5.2155567651	0.7655950109	12.3634885554
C9	3.3210971421	1.0932780184	11.3653180530
C10	3.4381315892	2.6266823847	9.5206816716
H11	5.4266115192	3.4150071640	9.1616710462
C12	6.8104199645	3.1201911199	13.6808466580
C13	6.4667253029	4.8731941819	12.0623138435
H14	2.7925809993	0.4270302787	12.0392346313
C15	2.6579829082	1.8137958051	10.3583117950
H16	3.0187918655	3.1589168315	8.6725211799
C17	6.6485462666	4.0442381068	14.7147434725
H18	7.0257221830	2.0814131014	13.9226551605
H19	6.4098305069	5.2124584699	11.0301082465
C20	6.3061723042	5.7943780652	13.0933416240
C21	1.1817524840	1.7862770291	10.2692315614
C22	6.3797495505	5.3873737211	14.4321210819
H23	6.7411488956	3.7121728284	15.7468484223
H24	6.1268130696	6.8398920876	12.8514673951
C25	0.4268565266	0.6998034845	10.7425392415
C26	0.4778082429	2.9036224072	9.7933888901
C27	6.1099907449	6.3785070076	15.5417655190
H28	0.8869859346	-0.2295498069	11.0655037503
C29	-0.9500049032	0.7911614238	10.8062941002
C30	-0.9013524100	2.9468916918	9.8730296150
H31	0.9862897426	3.7776059098	9.3999463547
N32	4.6270903572	6.5434447410	15.7123985054
H33	6.5152872232	7.3697542019	15.3226685744
H34	6.5080689733	6.0487169844	16.5048835461
N35	-1.5930790902	1.9163189455	10.4105680691
H36	-1.5664701081	-0.0208023032	11.1787112436
H37	-1.4786050420	3.8003699840	9.5307299835
C38	3.9360121360	5.5668575517	16.3464124929
C39	3.9811627502	7.5679378039	15.1103211273
C40	-3.0673318389	2.0606267464	10.6661038376
C41	2.5566896692	5.5568580753	16.3308279905
H42	4.5203105729	4.7956077010	16.8379424253
H43	4.5998180132	8.3384772669	14.6607636939
C44	2.5987372368	7.5971993954	15.0577838222
H45	-3.5311594377	1.1124358818	10.3797208124
H46	-3.4257207271	2.8372766698	9.9862587873
C47	-3.3318265511	2.3940570880	12.1182698678
C48	1.8554708149	6.5549921102	15.6322846331
H49	2.0456901483	4.7344706468	16.8200700755

H50	2.1235361162	8.4373963111	14.5621392397
C51	-3.5654108074	1.3576955373	13.0294939128
C52	-3.3505953066	3.7207311120	12.5721318369
C53	0.3937467713	6.4265294165	15.4296151077
H54	-3.5804108074	0.3254268376	12.6850277911
C55	-3.8083947256	1.6400736630	14.3712334560
C56	-3.6044629000	4.0122924146	13.9197118894
H57	-3.2002743785	4.5348752801	11.8632254802
C58	-0.4272426354	5.7367696068	16.3369895353
C59	-0.1999503473	6.9125116590	14.2531998212
H60	-3.9963394744	0.8307459157	15.0699224526
C61	-3.8292472969	2.9598833610	14.8148138043
C62	-3.6379226183	5.4384646357	14.4268550627
C63	-1.7488227415	5.4898929369	16.0187933944
H64	-0.0576101338	5.3850047572	17.2955118042
H65	0.3690009668	7.4700375238	13.5165061953
C66	-1.5232921427	6.6294298850	13.9745319968
H67	-4.0452826902	3.1722849029	15.8601226668
N68	-2.2678657203	5.8989198821	14.8360847225
H69	-4.2777499228	5.5349059579	15.3085455615
H70	-3.9932136940	6.1436863814	13.6713568689
H71	-2.4151066606	4.9531808805	16.6867223094
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C4	16.8716422401	14.7958226125	2.2486800082
C5	19.3917916227	15.0767049090	4.1421113133
H6	18.7059412791	17.0965885467	3.8139061327
H7	19.1245321756	16.2170409044	2.3408677407
H8	16.6016286019	17.0319002434	4.6908988138
C9	14.9719114097	15.8828763745	3.9019424442
C10	15.5949982438	14.3563834350	2.1467981046
H11	17.6806348643	14.3774163460	1.6562730477
C12	19.4040156898	15.1301316678	5.5400023727
C13	20.0471310038	14.0121383032	3.5136424701
H14	14.2794049874	16.3221659665	4.6131060082
C15	14.5169056579	14.8849731338	2.9557461524
H16	15.4130014603	13.5439718239	1.4506502202
C17	20.0496776663	14.1483757615	6.2858599859
H18	18.9055052302	15.9560151721	6.0487373412
H19	20.0678233127	13.9642250693	2.4244114177
C20	20.6849420099	13.0238704697	4.2600118692
C21	13.1983164578	14.4453470164	2.8633504291
C22	20.7002899286	13.0766661786	5.6583663155
H23	20.0562859260	14.2140758165	7.3741458304

H24	21.1929978789	12.2044640401	3.7507609936
C25	12.1279057859	14.9124465551	3.7215911378
C26	12.7496839492	13.4357802464	1.9255909037
C27	21.3049805021	11.9601374405	6.4658246415
H28	12.3095336495	15.7051639410	4.4411063014
C29	10.8775263014	14.3991448302	3.6811338773
C30	11.4915273356	12.9459457901	1.9152471140
H31	13.4407884526	13.0219124310	1.1982906843
N32	20.3182841891	10.9456542658	6.8821356904
H33	22.0827764810	11.4437763588	5.8888566382
H34	21.7726532615	12.3461861404	7.3802939401
N35	10.4827757503	13.4091454457	2.7720680462
H36	10.0843257040	14.7509616555	4.3368029559
H37	11.1768118481	12.1662723921	1.2248695666
C38	19.4115115060	11.3256138657	7.8901656148
C39	19.7700898635	10.1416826354	5.8656762397
C40	9.4835602024	12.4274769597	3.2282295251
C41	18.1278289652	10.9095674232	7.9251177655
H42	19.8391097984	11.9567460661	8.6677502110
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C44	18.4909912356	9.7009244146	5.8754021240
H45	8.6712137695	12.9937241539	3.7013288741
H46	9.0696381231	11.9377193309	2.3378665955
C47	10.0547105155	11.4052520805	4.1780591464
C48	17.5405581480	10.0697962090	6.9029526111
H49	17.5359663565	11.2196650907	8.7802213899
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C51	10.3462674027	11.7560059340	5.5036038097
C52	10.3895643417	10.1181389057	3.7467928661
C53	16.1940963511	9.7017030290	6.8968005029
H54	10.0929355191	12.7529598817	5.8621929966
C55	10.9577477156	10.8507066812	6.3626440509
C56	10.9940971884	9.2080295461	4.6132279938
H57	10.1710394893	9.8254472453	2.7196375521
C58	15.2606220489	10.1078398354	7.9185842584
C59	15.5835816579	8.8977147106	5.8649899392
H60	11.1886293245	11.1486511636	7.3849988711
C61	11.2905596999	9.5615183093	5.9318029286
H62	11.2429345658	8.2069910318	4.2593281458
C63	13.9643208258	9.7178197586	7.9192210841
H64	15.5833621426	10.7292035671	8.7468262520
H65	16.1568757778	8.5691204246	5.0042826485
C66	14.2843300564	8.5313233005	5.9064115329
C67	12.0180665129	8.6120771895	6.8527668311
N68	13.4453112661	8.8864364315	6.9456092426
H69	13.2691848579	10.0067438615	8.7026884741
H70	13.8219144288	7.9329944106	5.1273560865
H71	11.6081325270	8.6635378564	7.8685940976

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N73	15.2196072524	14.1555567282	7.3706652703
C74	15.2127565759	14.7085074597	8.7225373634
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C76	16.4171244295	13.7147986380	6.8179321902
C77	15.4855931817	13.6811444568	9.7942032416
H78	14.2350924959	15.1817535318	8.8739131950
H79	15.9707484935	15.5022378558	8.7680522065
H80	13.1319993881	14.0040950724	7.2632944217
C81	14.0649988734	12.8261930536	5.7350519274
C82	16.4706644623	12.9008418778	5.7382003601
H83	17.3147452537	14.0743216988	7.3118463779
C84	14.4715769283	12.8370304633	10.2657340437
C85	16.7814724171	13.4922359196	10.2841114935
H86	13.1003813164	12.5370577451	5.3339835116
C87	15.2838254360	12.3683983046	5.1090016116
H88	17.4618619689	12.6281632659	5.3831063915
C89	14.7495692822	11.8260063258	11.1796471841
H90	13.4536936031	12.9696148981	9.8986606890
H91	17.5831982393	14.1463371179	9.9387610158
C92	17.0620946208	12.4775549989	11.1971802392
C93	15.3008724040	11.4850749225	4.0316715480
C94	16.0540371296	11.6219327200	11.6511469945
H95	13.9468515906	11.1756462958	11.5271240240
H96	18.0815507521	12.3420749496	11.5611269127
C97	14.1075283370	10.8683139852	3.4920956885
C98	16.5092561209	11.0421501559	3.3662048805
C99	16.3875645884	10.4488751231	12.5391668751
H100	13.1273107603	11.1338296582	3.8750144367
C101	14.1402984762	9.9346494741	2.5156297746
C102	16.5050355648	10.1110250588	2.3829041844
H103	17.4734798861	11.4559121372	3.6494697498
N104	16.4800499879	9.1800829578	11.8029026015
H105	17.3497351516	10.6171211289	13.0405232821
H106	15.6304182979	10.3106763523	13.3204579843
N107	15.3282819960	9.5276760057	1.9136311841
H108	13.2410469365	9.4635930197	2.1241485806
H109	17.4130754213	9.7737262975	1.8888358900
C110	15.3149334468	8.4541482951	11.5544909972
C111	17.4981732257	9.0415988169	10.8546144899
C112	15.3841891343	8.3591003921	1.0550702797
C113	15.1922041528	7.5954320247	10.5161186365
H114	14.5213319197	8.6047476197	12.2824227062
H115	18.3698696129	9.6687041921	11.0240868405
C116	17.4159887271	8.1913702637	9.8062853368
H117	15.9514725590	8.6067970120	0.1444557593
H118	14.3567505845	8.1450503870	0.7350425459
C119	16.0122496999	7.1377311863	1.6918741435

C120	16.2354663524	7.3983063611	9.5290277229
H121	14.2536715713	7.0543733014	10.4371096262
H122	18.2652287826	8.1677935509	9.1299072370
C123	15.4445620722	6.5082127853	2.8059353754
C124	17.2017765712	6.6252608217	1.1643008625
C125	16.0843932575	6.6223177084	8.3848643599
H126	14.5214493242	6.9057066729	3.2308639781
C127	16.0339610239	5.3753808848	3.3756961660
C128	17.8021522988	5.5004908668	1.7220594157
H129	17.6541944757	7.1155455508	0.3020950281
C130	14.8625636110	5.9238804226	8.0351256307
C131	17.1141241948	6.4749712902	7.3745236750
C132	17.2168308173	4.8767270417	2.8201125041
C133	15.4308700343	4.6759006831	4.5698072143
H134	18.7256475081	5.1093826971	1.3009814021
C135	14.6707406976	5.3570975723	6.8207613678
H136	14.0308685381	5.8840117268	8.7324994935
H137	18.1076209688	6.8813428498	7.5378367342
C138	16.8821073661	5.8910438683	6.1762824386
H139	17.6775970017	3.9925097156	3.2592345083
N140	15.6330801504	5.3953363253	5.8235626558
H141	15.8489088203	3.6578901576	4.6359217758
H142	14.3480618457	4.5638135686	4.4420194922
H143	13.7425511600	4.8633893182	6.5448377899
H144	17.6450153842	5.8197852144	5.4070597026

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N1	17.4747149806	15.8483762577	2.7821240609
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C3	16.5224669225	16.2505807800	3.7036334242
C4	17.1062776352	14.8573650247	1.8870478821
C5	19.5824987864	15.1143751811	3.8585564962
H6	18.9543724094	17.1388977590	3.4538925003
H7	19.3721071967	16.2059016505	2.0119041577
H8	16.8590689307	16.9923458553	4.4226944289
C9	15.2536657230	15.7718638548	3.6937462229
C10	15.8511149289	14.3463873287	1.8471895404
H11	17.8862691341	14.5398400303	1.2006334429
C12	19.6238340537	15.2513333194	5.2503713012
C13	20.1313507740	13.9615683172	3.2856850598
H14	14.5771612077	16.1620384189	4.4486475967
C15	14.8056280789	14.7714501681	2.7506031295
H16	15.6565654702	13.5922468210	1.0922082447
C17	20.1802105269	14.2548389157	6.0475832533
H18	19.2212969796	16.1526663873	5.7126802577
H19	20.1348269664	13.8497725644	2.2017184209
C20	20.6831068269	12.9627495864	4.0826588469
C21	13.5033307856	14.2584517442	2.7228671359

C22	20.7084518516	13.0912090322	5.4755269141
H23	20.2122338813	14.3819454655	7.1297604305
H24	21.1076943544	12.0729920446	3.6182229877
C25	12.4520078547	14.6937890598	3.6155527231
C26	13.0664186305	13.2286587123	1.8066061804
C27	21.1779247147	11.9514078094	6.3413740000
H28	12.6271343667	15.4987591734	4.3218712995
C29	11.2133765232	14.1448558963	3.6113220845
C30	11.8218783172	12.6946021993	1.8444024163
H31	13.7505912307	12.8241542711	1.0661413758
N32	20.0590842460	11.0714704094	6.7114804082
H33	21.9236419377	11.3398408816	5.8207138535
H34	21.6323549531	12.3146482484	7.2704721921
N35	10.8413256722	13.1401616198	2.7241792638
H36	10.4247570148	14.4835439098	4.2782141315
H37	11.5084836450	11.8980926483	1.1742063870
C38	19.2023985345	11.4635084684	7.7319871177
C39	19.5464122944	10.1973982641	5.7616376817
C40	9.7387776675	12.2400165152	3.0935167593
C41	17.9298316223	11.0058213985	7.8258697865
H42	19.6391139809	12.1368033215	8.4664174857
H43	20.2450458298	9.9062145124	4.9819101633
C44	18.2791011206	9.7160487459	5.8243674428
H45	8.9233713689	12.8648171384	3.4789889582
H46	9.3814987976	11.7566920945	2.1767414316
C47	10.1635768471	11.2141750204	4.1153780769
C48	17.3499750800	10.1170342330	6.8514348898
H49	17.3550054672	11.3281461976	8.6865000798
H50	17.9835431026	9.0013330686	5.0623700131
C51	10.3436785661	11.5878316668	5.4549195806
C52	10.4750909238	9.9020398757	3.7468949303
C53	16.0088791876	9.6966457157	6.8995549781
H54	10.0801083282	12.5961088756	5.7722595278
C55	10.8565618913	10.6895569039	6.3835335357
C56	10.9791545443	8.9979712962	4.6817184092
H57	10.3230702075	9.5853758638	2.7147201181
C58	15.0903913188	10.1149143761	7.9246491687
C59	15.4227290426	8.8115546377	5.9306589415
H60	11.0007987944	11.0059559317	7.4164811818
C61	11.1949857657	9.3830794476	6.0088090925
H62	11.2124465789	7.9778459570	4.3745973325
C63	13.8111370367	9.6669491025	7.9803597398
H64	15.4034733876	10.7982740008	8.7079993838
H65	15.9932141953	8.4518753079	5.0798201778
C66	14.1401630522	8.3890098641	6.0267848267
C67	11.8827934451	8.4655708908	6.9868086556
N68	13.3156338976	8.7565777672	7.0692271633
H69	13.1203266668	9.9669157115	8.7636489018

H70	13.6923841051	7.7161400916	5.3016088387
H71	11.4672002112	8.5678439861	7.9955400188
H72	11.7694268543	7.4154330721	6.6890208117
N73	15.1732836380	14.3061392004	7.6717043774
C74	15.2410880394	14.8380972836	9.0401177751
C75	14.0057991369	13.7225403362	7.2237161656
C76	16.3350785949	14.0204015064	6.9801937756
C77	15.4958388412	13.7448677363	10.0472437567
H78	14.2918398791	15.3492930029	9.2381158744
H79	16.0353753305	15.5926595415	9.0664539365
H80	13.1112145349	13.9829213315	7.7840250605
C81	13.9789800840	12.9041489085	6.1396776665
C82	16.3475903875	13.2246132772	5.8785590901
H83	17.2363107396	14.4841281314	7.3717361659
C84	14.4449233063	12.9357206540	10.4992504000
C85	16.7922061904	13.4545260060	10.4809898778
H86	13.0100572179	12.5238887188	5.8361158392
C87	15.1638510944	12.5699359741	5.3975019779
H88	17.3078156947	13.0769178959	5.3929881779
C89	14.6877892843	11.8542164400	11.3391911467
H90	13.4247069582	13.1566250216	10.1859577583
H91	17.6214572409	14.0819549671	10.1534472957
C92	17.0350924571	12.3723206998	11.3248075718
C93	15.1558216109	11.6550418538	4.3230552987
C94	15.9896492537	11.5491959875	11.7559107544
H95	13.8565232668	11.2360157889	11.6776167367
H96	18.0526432118	12.1630315139	11.6559519860
C97	13.9834199933	10.9226368919	3.9390066824
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C99	16.2739121044	10.3135506069	12.5736707856
H100	13.0331380283	11.0806212914	4.4381395403
C101	14.0023149848	9.9848401468	2.9563300260
C102	16.2965071869	10.3852247022	2.5641499568
H103	17.2633312817	11.8340329695	3.7168577145
N104	16.3567285385	9.0969121966	11.7574776350
H105	17.2255212846	10.4254643158	13.1077411553
H106	15.4930211810	10.1466565278	13.3243098496
N107	15.1429475258	9.6931498609	2.2456457023
H108	13.1180773176	9.4193570884	2.6761974763
H109	17.1709836300	10.1298782752	1.9722815324
C110	15.2041892946	8.3678980206	11.4774437075
C111	17.4016982625	8.9764349680	10.8412836791
C112	15.1829724348	8.5901101163	1.2866162924
C113	15.1154053403	7.5155296121	10.4297058471
H114	14.3911306642	8.5076197493	12.1856115894
H115	18.2697813465	9.5967920132	11.0495675589
C116	17.3518236024	8.1377536155	9.7812720719
H117	15.6583876587	8.9481627108	0.3641256056

H118	14.1441533042	8.3457333621	1.0341462526
C119	15.9162975555	7.3691114778	1.7948032125
C120	16.1863347116	7.3344375862	9.4694118681
H121	14.1816465002	6.9720041892	10.3193938656
H122	18.2244062263	8.1159767609	9.1350640305
C123	15.4278093488	6.6129855134	2.8658776515
C124	17.1057920486	6.9734313781	1.1752416053
C125	16.0802281567	6.5513059266	8.3241653123
H126	14.5039233325	6.9175876981	3.3604419303
C127	16.0971173228	5.4677100566	3.3090571102
C128	17.7851973715	5.8380823053	1.6078749545
H129	17.4941913177	7.5598653964	0.3430532426
C130	14.8876981387	5.8157816441	7.9461737091
C131	17.1406170387	6.4260516964	7.3427312511
C132	17.2797679189	5.0882728054	2.6667124351
C133	15.5824238021	4.6445489445	4.4674766712
H134	18.7094049516	5.5371968804	1.1198933384
C135	14.7378289199	5.2516023899	6.7236547669
H136	14.0469730902	5.7369331013	8.6299407239
H137	18.1280022816	6.8292952381	7.5420652879
C138	16.9516179308	5.8475706915	6.1353122344
H139	17.8059859421	4.1965861916	3.0063880516
N140	15.7214128714	5.3293911655	5.7471818886
H141	16.1120428967	3.6778070910	4.4848537438
H142	14.5173776364	4.4197220546	4.3394095160
H143	13.8343021621	4.7245494438	6.4276998683
H144	17.7400285144	5.7798192891	5.3913335563

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C3	16.7163884801	16.1979961583	3.8101810669
C4	17.2904355834	14.8579619348	1.9505008718
C5	19.6211745454	14.9139267850	4.0787225651
H6	19.2104519498	16.9917901789	3.6349750354
H7	19.6296586920	16.0157790889	2.2182185206
H8	17.0552786138	16.9227248324	4.5457781150
C9	15.4403221296	15.7347842855	3.7784659539
C10	16.0288858850	14.3614643019	1.8906706122
H11	18.0642215895	14.5671754263	1.2455556187
C12	19.6411964352	15.0755698745	5.4680979230
C13	19.9925859859	13.6738544687	3.5439281711
H14	14.7597173898	16.1242082906	4.5299762098
C15	14.9943963616	14.7604852312	2.8134575401
H16	15.8205776969	13.6552488169	1.0941090282
C17	19.9923234419	14.0164224588	6.3020329696
H18	19.3841217762	16.0429389457	5.8995647287
H19	20.0163947877	13.5383701645	2.4631649541

C20	20.3387093279	12.6153668781	4.3766184281
C21	13.6805453026	14.2609444075	2.7665599454
C22	20.3283738805	12.7675187275	5.7682731342
H23	20.0128716307	14.1626518416	7.3825519636
H24	20.6283699015	11.6592159062	3.9418234463
C25	12.6336991181	14.6979351981	3.6575312802
C26	13.2386639802	13.2721277082	1.8147119456
C27	20.5578784606	11.5799410726	6.6655378556
H28	12.8226511181	15.4622696236	4.4036248709
C29	11.3708787441	14.2047097949	3.5960962168
C30	11.9667172821	12.7954344945	1.7959329557
H31	13.9259329860	12.8632098868	1.0797783038
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H33	21.2687358606	10.8715228562	6.2276345511
H34	20.9465103387	11.8811714657	7.6442960443
N35	10.9911177847	13.2611790261	2.6579995942
H36	10.5791725645	14.5483753101	4.2559830379
H37	11.6372960198	12.0403094097	1.0869645995
C38	18.3904774571	11.3187370791	7.8158759618
C39	18.8516677463	9.9345963918	5.9663537234
C40	9.7515655276	12.4947402779	2.8590265564
C41	17.1040187801	10.8745267704	7.8595420853
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C44	17.5711860418	9.4724010439	5.9661192455
H45	8.9830883029	13.1980731962	3.2007980626
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C47	9.9534664476	11.3783288858	3.8522807397
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H49	16.4763957951	11.2797058196	8.6486924590
H50	17.3224376793	8.7258888997	5.2186187229
C51	9.9519737376	11.6501860493	5.2273340744
C52	10.2404992909	10.0763847080	3.4298959389
C53	15.2514244252	9.4673085268	6.9349177482
H54	9.6936086473	12.6484605754	5.5793147117
C55	10.2729900808	10.6596365708	6.1486780997
C56	10.5552503760	9.0809728436	4.3540767240
H57	10.2159460034	9.8393555798	2.3659534612
C58	14.2774721264	9.9003636527	7.8977221543
C59	14.7469178242	8.5190104228	5.9930201939
H60	10.2700054509	10.8912322456	7.2135341193
C61	10.5970602400	9.3653698487	5.7230552508
H62	10.7708125517	8.0695140324	4.0080981727
C63	12.9903016902	9.4571709156	7.8737326407
H64	14.5459078388	10.5913017514	8.6895929137
H65	15.3978820473	8.0910356055	5.2368136928
C66	13.4507975941	8.1033147235	6.0007105808
C67	11.1060590092	8.3482763895	6.7111464783

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H69	12.2463033275	9.7751648625	8.5989700068
H70	13.0594479132	7.3840278115	5.2855468708
H71	10.6068815587	8.4343530471	7.6819086039
H72	10.9623637241	7.3244870639	6.3485247445
N73	15.2521177074	14.4014206136	7.6560120633
C74	15.4199008590	14.9981118139	8.9942564537
C75	14.0650945563	13.7857661367	7.3229933037
C76	16.3587255844	14.1178522424	6.8897409160
C77	15.8125288147	13.9401179166	9.9928740712
H78	14.4703254565	15.4753312574	9.2599759974
H79	16.1796296937	15.7837670121	8.9188165315
H80	13.2121649128	14.0530700256	7.9408401060
C81	13.9718476416	12.9249580944	6.2734707954
C82	16.3063582739	13.2738241587	5.8228370825
H83	17.2733828318	14.6252813512	7.1818598087
C84	14.8381322436	13.0976200064	10.5436592866
C85	17.1548119452	13.7005965149	10.3052238723
H86	12.9911144776	12.5129367325	6.0617862182
C87	15.1056646013	12.5824245223	5.4595596096
H88	17.2285442630	13.1407324750	5.2623444428
C89	15.1987927687	12.0304117335	11.3585281111
H90	13.7850275506	13.2853800212	10.3357785523
H91	17.9247642106	14.3643778705	9.9106515930
C92	17.5166457962	12.6295735663	11.1211599982
C93	15.0415835087	11.6342286317	4.4071861150
C94	16.5454837371	11.7705438858	11.6463039186
H95	14.4243288558	11.3933842144	11.7849201398
H96	18.5672343834	12.4599249243	11.3576338203
C97	13.8524951501	10.9025034452	4.0878458525
C98	16.1665665805	11.3034985793	3.5757938102
C99	16.9316773790	10.5360745529	12.4212703710
H100	12.9169561937	11.0816215355	4.6129785144
C101	13.8405069629	9.9240922699	3.1394506554
C102	16.1055709500	10.3275527030	2.6296983053
H103	17.1089758136	11.8331585932	3.6768534611
N104	16.9549588168	9.3450086931	11.5575512411
H105	17.9266790247	10.6429141829	12.8661226271
H106	16.2226503741	10.3371628078	13.2330065287
N107	14.9542015056	9.6039578678	2.4080645990
H108	12.9484844697	9.3483304645	2.9136703221
H109	16.9506881749	10.0673699290	1.9992998095
C110	15.7743040592	8.6904465372	11.2542421197
C111	18.0409300072	9.1114905396	10.7331468199
C112	14.9624927008	8.4681537823	1.4738857338
C113	15.6728577993	7.8244291034	10.2133980121
H114	14.9443598447	8.8941471239	11.9252752559
H115	18.9484702376	9.6468550071	10.9990863964

C116	17.9822501708	8.2518600239	9.6834928991
H117	15.2398079592	8.8406600782	0.4800051340
H118	13.9323948882	8.1033230313	1.4060325861
C119	15.9124243203	7.3685717875	1.8908701965
C120	16.7739314905	7.5557680491	9.3218144908
H121	14.7138968514	7.3352073202	10.0753677760
H122	18.8946162539	8.1149237860	9.1105166820
C123	15.6166362639	6.4951301898	2.9442357704
C124	17.1266774355	7.2238005049	1.2124029930
C125	16.6699667038	6.7150323544	8.1974931381
H126	14.6593005102	6.5808567709	3.4628653558
C127	16.5168660291	5.4929073700	3.3256128266
C128	18.0276418805	6.2275452361	1.5774438594
H129	17.3586250554	7.8931872026	0.3846528495
C130	15.4596604217	6.0246845257	7.8314994335
C131	17.7577425075	6.4799891643	7.2802725154
C132	17.7234249701	5.3686610566	2.6293303246
C133	16.2281902384	4.5563629473	4.4779612575
H134	18.9667244048	6.1190204462	1.0403481912
C135	15.3450407429	5.3191357641	6.6746042267
H136	14.5781320219	6.0726066935	8.4630815463
H137	18.7457775839	6.8855845004	7.4726721438
C138	17.6009223796	5.7674636549	6.1352785143
H139	18.4243849275	4.5840272165	2.9125494554
N140	16.3902845572	5.1992624871	5.7861410379
H141	16.8997770701	3.6893119182	4.4227176572
H142	15.2029863522	4.1756108678	4.4331866324
H143	14.4268513078	4.8163854083	6.3838377467
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C4	17.2785933192	14.6597712584	1.9301931296
C5	19.6269508419	14.8534085795	4.0470222862
H6	19.1579021659	16.9015170662	3.5022449913
H7	19.5933475778	15.8676102435	2.1313053262
H8	17.0256453577	16.8575657350	4.4066752516
C9	15.4006794005	15.6580902734	3.6629454456
C10	16.0027954553	14.1835079611	1.8588935739
H11	18.0633438446	14.3239415976	1.2581447254
C12	19.6219768267	15.0667791454	5.4302898104
C13	20.0493757170	13.6092412203	3.5631497417
H14	14.7070135756	16.1069456584	4.3673017473
C15	14.9711743800	14.6531621845	2.7379275011
H16	15.7973844649	13.4540678302	1.0839449466
C17	19.9847097606	14.0455988482	6.3076157593

H18	19.3339553060	16.0415154222	5.8242786615
H19	20.1002499444	13.4365087622	2.4885057967
C20	20.4081130056	12.5896172598	4.4395813235
C21	13.6295444696	14.1780395047	2.6819916940
C22	20.3572976708	12.7858409861	5.8245383835
H23	19.9821866832	14.2319037719	7.3821380443
H24	20.7360054559	11.6295180531	4.0422694253
C25	12.5921654628	14.6675004329	3.5416022286
C26	13.1941056465	13.1846773787	1.7478464942
C27	20.5843545505	11.6289231318	6.7640328211
H28	12.7795070844	15.4625228488	4.2547682544
C29	11.3222961627	14.1773868384	3.4903475598
C30	11.9129130335	12.7156934383	1.7364130026
H31	13.8747516090	12.7696520190	1.0109960736
N32	19.3158139954	10.9011687035	6.9800118288
H33	21.3088976958	10.9134060108	6.3615145366
H34	20.9497411079	11.9607935653	7.7416086352
N35	10.9591271156	13.1956102024	2.5989484432
H36	10.5283870209	14.5495452096	4.1315657669
H37	11.5755611495	11.9563714078	1.0360327884
C38	18.4132200110	11.3483473379	7.9100666344
C39	18.8858251021	9.9812203379	6.0538454115
C40	9.6961125007	12.4559623301	2.7993881839
C41	17.1259350568	10.8990308766	7.9471382689
H42	18.7930882980	12.0742024959	8.6230643841
H43	19.6385057816	9.6444709975	5.3465434789
C44	17.6046567424	9.5168475031	6.0441461273
H45	8.9408554795	13.1785772943	3.1262855781
H46	9.3840904487	12.0559520858	1.8292692203
C47	9.9067956810	11.3619257574	3.8171062673
C48	16.6220427038	9.9608849384	6.9922211978
H49	16.4955419959	11.2935009704	8.7393633980
H50	17.3580195593	8.7811368659	5.2865554799
C51	9.9075324881	11.6633834456	5.1856261646
C52	10.2133158972	10.0571564426	3.4186413109
C53	15.2733417524	9.5062485109	6.9911081997
H54	9.6339545417	12.6639892869	5.5192404711
C55	10.2519605944	10.6972720611	6.1258221472
C56	10.5520049564	9.0870825045	4.3619794272
H57	10.1849165622	9.7966849403	2.3604790639
C58	14.2944792657	9.9369331960	7.9495269260
C59	14.7705030021	8.5704281100	6.0365897994
H60	10.2476105801	10.9515867864	7.1853769135
C61	10.6000115334	9.4012879645	5.7243674663
H62	10.7797444842	8.0722481544	4.0344980459
C63	13.0011065325	9.5084333511	7.9068974005
H64	14.5606340483	10.6201185668	8.7491758409
H65	15.4231589469	8.1254441642	5.2914410548

C66	13.4687997268	8.1652912490	6.0301662628
C67	11.1182200087	8.4052202991	6.7302807708
N68	12.5634988591	8.6179064576	6.9554176498
H69	12.2528226277	9.8274564414	8.6274345817
H70	13.0790442950	7.4512114744	5.3089095323
H71	10.6189832879	8.5034451903	7.6994239885
H72	10.9825652969	7.3747334644	6.3847652130
N73	15.2710110788	14.3805358374	7.7231307710
C74	15.4476195215	14.9707278321	9.0657544885
C75	14.0721772164	13.8043882632	7.3723737323
C76	16.3672398783	14.1160600070	6.9416870755
C77	15.8433148469	13.9042906969	10.0571945966
H78	14.5007661605	15.4468291241	9.3379217248
H79	16.2073576453	15.7559983006	8.9910578327
H80	13.2238627621	14.0711771279	7.9969474087
C81	13.9637157507	12.9706860580	6.2996076766
C82	16.3008432840	13.2988626928	5.8523174626
H83	17.2892557712	14.6034960419	7.2448801833
C84	14.8703608778	13.0564754222	10.6025028260
C85	17.1851469754	13.6736161413	10.3772042438
H86	12.9765562571	12.5778038139	6.0795921110
C87	15.0931669997	12.6253560939	5.4831230347
H88	17.2202315933	13.1669973261	5.2875814812
C89	15.2339753473	11.9841557726	11.4104031020
H90	13.8163103984	13.2418030817	10.3971646880
H91	17.9534926377	14.3468620496	9.9955198932
C92	17.5505012827	12.5968087193	11.1858391342
C93	15.0246951832	11.6825537638	4.4199321630
C94	16.5816996144	11.7259345602	11.6942435781
H95	14.4602928683	11.3416448882	11.8301277746
H96	18.6010936248	12.4317809122	11.4252111273
C97	13.8367198196	10.9554661207	4.0933913138
C98	16.1536514239	11.3504211949	3.5972959037
C99	16.9711111756	10.4750837515	12.4441417447
H100	12.9014068094	11.1264818497	4.6220808308
C101	13.8259779468	9.9885104557	3.1298928837
C102	16.0918843396	10.3908249069	2.6341214169
H103	17.1004926440	11.8658622597	3.7158595362
N104	16.9755898695	9.3152900635	11.5303813084
H105	17.9714645852	10.5591204920	12.8794735655
H106	16.2683169791	10.2517524085	13.2540395755
N107	14.9390699060	9.6793404778	2.3963336434
H108	12.9341333454	9.4153181139	2.8963728063
H109	16.9398708371	10.1368076217	2.0050405948
C110	15.8019757744	8.6557488044	11.2519911890
C111	18.0639688384	9.0724256697	10.7272021085
C112	14.9538042943	8.5533906309	1.4440064562
C113	15.6946828569	7.7911545311	10.2048031594

H114	14.9766990713	8.8539125696	11.9300809022
H115	18.9756466964	9.5970789809	10.9995659563
C116	18.0011881544	8.2119342816	9.6709544909
H117	15.2361800995	8.9425618047	0.4583522793
H118	13.9256875642	8.1859903299	1.3658332743
C119	15.9073994426	7.4579212160	1.8607490227
C120	16.7885458396	7.5397749215	9.3125662151
H121	14.7379959017	7.2975166722	10.0757377701
H122	18.9151164468	8.0634851996	9.1035622309
C123	15.5983156514	6.5691031953	2.8977918884
C124	17.1374208502	7.3359836092	1.2068324610
C125	16.6715774920	6.7081359450	8.1620246048
H126	14.6263611513	6.6390886591	3.3906641943
C127	16.5011525060	5.5715309187	3.2858621065
C128	18.0410456198	6.3448023266	1.5799272425
H129	17.3799748649	8.0164961701	0.3911146518
C130	15.4568322606	6.0436618972	7.7990509719
C131	17.7530918580	6.4843893765	7.2473707571
C132	17.7241481774	5.4688729080	2.6142191686
C133	16.1966721004	4.6164796323	4.4174118507
H134	18.9921138479	6.2524463323	1.0612625297
C135	15.3309272228	5.3538031768	6.6273435424
H136	14.5793899101	6.0861084554	8.4364139999
H137	18.7472539443	6.8697787547	7.4447735254
C138	17.5839324376	5.7897469591	6.0880863786
H139	18.4271892287	4.6872047360	2.9001613140
N140	16.3699228326	5.2444324217	5.7410936957
H141	16.8584827760	3.7437056941	4.3617350758
H142	15.1664750537	4.2511552822	4.3707651462
H143	14.4077288660	4.8618286575	6.3342523511
H144	18.3945183271	5.6292475455	5.3837627940

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N1	17.6463264673	15.6984714787	2.8448019928
C2	19.0907562210	15.9387554031	3.0830294473
C3	16.7204513379	16.1615914792	3.7368120689
C4	17.2528809051	14.8034781438	1.8881933178
C5	19.6208861908	14.8645356380	4.0021681577
H6	19.1948813829	16.9406683994	3.5110360555
H7	19.5898212311	15.9305813416	2.1087739965
H8	17.0768638470	16.8924128070	4.4577118317
C9	15.4178657750	15.7409053125	3.6993788863
C10	15.9644431882	14.3495201340	1.8190608105
H11	18.0176789767	14.4949322306	1.1807968091
C12	19.6577493913	15.0535962469	5.3883794543
C13	19.9893417188	13.6160618717	3.4853242877
H14	14.7439080362	16.1764401868	4.4297141884
C15	14.9713839718	14.7772592692	2.7507579418

H16	15.7296698705	13.6700382493	1.0075975975
C17	20.0104430954	14.0048500533	6.2384126323
H18	19.4162670167	16.0305443375	5.8071962298
H19	20.0107509261	13.4608743802	2.4068713395
C20	20.3388585187	12.5696381331	4.3347076872
C21	13.6157648069	14.2896785301	2.7195741125
C22	20.3302810489	12.7431589758	5.7240925258
H23	20.0469631368	14.1749992728	7.3148155959
H24	20.6317026363	11.6097250772	3.9107211678
C25	12.6046340118	14.7752958895	3.6016680229
C26	13.1774895332	13.3014867875	1.7921533596
C27	20.5745921674	11.5689568823	6.6407014154
H28	12.8002208610	15.5748940438	4.3072979717
C29	11.3334035879	14.2723034844	3.5778735202
C30	11.8950923195	12.8203277426	1.8104444395
H31	13.8430120963	12.8913581803	1.0386636420
N32	19.3065100104	10.8386519083	6.8806128751
H33	21.2850103723	10.8558705212	6.2106635965
H34	20.9658109252	11.8843720373	7.6132420363
N35	10.9691858305	13.2896722943	2.6984472994
H36	10.5500563951	14.6383479508	4.2357964294
H37	11.5463946566	12.0626280916	1.1137586093
C38	18.4323133845	11.2658487942	7.8415469931
C39	18.8755364182	9.8943601178	5.9846421988
C40	9.6931028222	12.5592885573	2.8961612880
C41	17.1533988641	10.7914528653	7.9223504475
H42	18.8191308368	12.0051289489	8.5367590351
H43	19.6164666969	9.5587525703	5.2642737409
C44	17.6009647868	9.4058176496	6.0158912024
H45	8.9535088725	13.2843154237	3.2505967340
H46	9.3667053374	12.1886513702	1.9196285733
C47	9.9159678447	11.4414071883	3.8864867958
C48	16.6388641288	9.8464499381	6.9829990555
H49	16.5387880845	11.1830212361	8.7284069183
H50	17.3469467404	8.6601596661	5.2701710467
C51	9.9354455466	11.7122783035	5.2611548644
C52	10.2011202598	10.1413984766	3.4558092520
C53	15.2813628786	9.3982965051	6.9983447711
H54	9.6734419687	12.7067949853	5.6216020742
C55	10.2766220770	10.7203802666	6.1767467664
C56	10.5365713759	9.1455439713	4.3748166482
H57	10.1538646400	9.9017464629	2.3934899018
C58	14.3175894039	9.8387890780	7.9638221994
C59	14.7608202662	8.4801057326	6.0390978848
H60	10.2796581616	10.9509331879	7.2417003110
C61	10.6027607510	9.4288989833	5.7435311271
H62	10.7412314810	8.1345420687	4.0216014926
C63	13.0124980944	9.4380880162	7.9185362634

H64	14.5979348809	10.5119589498	8.7671881812
H65	15.3990482383	8.0459079987	5.2751260483
C66	13.4472753344	8.1057021621	6.0285861588
C67	11.1012167528	8.3979392620	6.7277241713
N68	12.5556235759	8.5791908075	6.9516859323
H69	12.2729268128	9.7633961049	8.6454014936
H70	13.0390287957	7.4110097647	5.2982554664
H71	10.6083969288	8.4853361632	7.7009214876
H72	10.9463237920	7.3776542490	6.3621075291
N73	15.2353219619	14.3566644430	7.6468214250
C74	15.3991274654	14.9540176110	8.9934954601
C75	14.0403000063	13.7892458511	7.2819503484
C76	16.3287922901	14.1299398244	6.8558944942
C77	15.8004577373	13.8954931586	9.9941176797
H78	14.4457505682	15.4221455106	9.2581837937
H79	16.1504233156	15.7467352781	8.9173745308
H80	13.1897994137	14.0359778580	7.9119976152
C81	13.9381940179	12.9761970622	6.1898660923
C82	16.2699621461	13.3339749936	5.7470833550
H83	17.2474262216	14.6175143356	7.1694397527
C84	14.8274475489	13.0688299557	10.5702663428
C85	17.1440029002	13.6666030883	10.3093138397
H86	12.9557209231	12.5727440602	5.9686611060
C87	15.0694483023	12.6565991098	5.3699314203
H88	17.1911832956	13.2186192534	5.1811228384
C89	15.1925337428	12.0138006711	11.4017165957
H90	13.7719685082	13.2576373715	10.3758750166
H91	17.9136213235	14.3283235717	9.9105127834
C92	17.5114312924	12.6071984787	11.1409279912
C93	15.0145155541	11.7035079626	4.3062545447
C94	16.5412985892	11.7550247154	11.6783745415
H95	14.4179797696	11.3902351266	11.8477816894
H96	18.5632407731	12.4452550724	11.3769667569
C97	13.8395280592	10.9521068116	3.9965624826
C98	16.1458383613	11.3782381942	3.4888016309
C99	16.9305344596	10.5176846983	12.4533306237
H100	12.8990845568	11.1224165669	4.5140805423
C101	13.8516075243	9.9463380331	3.0704066504
C102	16.1054687328	10.3784877619	2.5617934675
H103	17.0811312261	11.9194869181	3.5866710278
N104	16.9342668698	9.3507409304	11.5370172338
H105	17.9307827123	10.6002808376	12.8878479248
H106	16.2247177065	10.2978463075	13.2605650920
N107	14.9751132321	9.6247058704	2.3648232302
H108	12.9713216159	9.3473162874	2.8570761343
H109	16.9571415520	10.1244812599	1.9375433989
C110	15.7690516032	8.6860310075	11.2729187408
C111	18.0329701782	9.0925751670	10.7668668240

C112	15.0144147107	8.4497850572	1.4625462108
C113	15.6713738729	7.8002189521	10.2354809259
H114	14.9385928410	8.8916992250	11.9425970927
H115	18.9441814862	9.6150500186	11.0454680368
C116	17.9816328653	8.2096306854	9.7208574341
H117	15.2990145822	8.8037873704	0.4650165512
H118	13.9917291649	8.0664266132	1.3940514913
C119	15.9808390993	7.3893254821	1.9362452982
C120	16.7740234372	7.5453654878	9.3667143931
H121	14.7204666701	7.2942992050	10.1133209008
H122	18.9040304171	8.0458453574	9.1729820541
C123	15.6490098170	6.4855549537	2.9545667757
C124	17.2444300982	7.3076266245	1.3417242250
C125	16.6676045160	6.6841274309	8.2133944624
H126	14.6511090559	6.5185305736	3.3975713095
C127	16.5643219012	5.5125960989	3.3793945213
C128	18.1589205001	6.3417905871	1.7525349414
H129	17.5038417196	7.9950822826	0.5369435663
C130	15.4600334373	6.0261707568	7.8521961791
C131	17.7653927493	6.4433194710	7.3340676818
C132	17.8200341198	5.4491142477	2.7654056212
C133	16.2414231843	4.5485704069	4.4975076579
H134	19.1341563212	6.2783180020	1.2764538876
C135	15.3508726848	5.3131946695	6.6848350667
H136	14.5738513543	6.0755693834	8.4760447942
H137	18.7606782019	6.8168342472	7.5473978686
C138	17.6119052738	5.7231991176	6.1824860418
H139	18.5304616659	4.6830359449	3.0747025573
N140	16.4037453172	5.1855757030	5.8296548000
H141	16.9045194953	3.6770610619	4.4601092409
H142	15.2109603988	4.1861590086	4.4458997878
H143	14.4306321902	4.8188546687	6.3858000658
H144	18.4360303981	5.5413663611	5.4993729453

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C4	17.2451501058	14.8386587225	1.8634236317
C5	19.6139837349	14.8709354562	3.9928521489
H6	19.1894719470	16.9516413806	3.5004232738
H7	19.5831913609	15.9407022562	2.0969194699
H8	17.0718538537	16.9215153586	4.4332584816
C9	15.3977852637	15.7970864710	3.6527232141
C10	15.9441206819	14.4068751196	1.7762259641
H11	18.0120795312	14.5196838864	1.1624063626
C12	19.6568287143	15.0639211782	5.3782929505
C13	19.9847746708	13.6240899523	3.4738174169

H14	14.7214673021	16.2407478184	4.3774479405
C15	14.9598166040	14.8456942331	2.6986528693
H16	15.7110447073	13.7320923598	0.9599932243
C17	20.0157360674	14.0166613008	6.2284510951
H18	19.4182877160	16.0414848942	5.7973513139
H19	20.0071871367	13.4678941743	2.3955626644
C20	20.3397415758	12.5791300078	4.3236860147
C21	13.5870562446	14.3487814508	2.6656419480
C22	20.3337528789	12.7551791563	5.7126845213
H23	20.0603012459	14.1896554719	7.3042153166
H24	20.6360837193	11.6203753056	3.8994344574
C25	12.5908146330	14.8238073830	3.5566020351
C26	13.1612681472	13.3614631423	1.7431337649
C27	20.5758605715	11.5788076415	6.6296927914
H28	12.7815250970	15.6263665267	4.2605143299
C29	11.3229030774	14.2962198634	3.5534220861
C30	11.8828540862	12.8557178877	1.7812505017
H31	13.8219647819	12.9634080151	0.9787595255
N32	19.2956727177	10.8550762811	6.8582478954
H33	21.2828658780	10.8605374137	6.2032535152
H34	20.9612155782	11.8884706817	7.6063486466
N35	10.9746548169	13.3029010132	2.6901913680
H36	10.5436832936	14.6525447417	4.2220735920
H37	11.5361973093	12.0938443158	1.0874768041
C38	18.4196178102	11.2907979565	7.8107463378
C39	18.8728506636	9.9082932960	5.9652417966
C40	9.6926763859	12.5657195446	2.8874350589
C41	17.1350202479	10.8230100478	7.8824660027
H42	18.8076132966	12.0264463821	8.5094799370
H43	19.6211142423	9.5636459053	5.2564408424
C44	17.5934579393	9.4229992183	5.9872178609
H45	8.9546765339	13.2917363925	3.2421891493
H46	9.3704685108	12.1979850914	1.9088954691
C47	9.9188129574	11.4464691371	3.8788143887
C48	16.6291287636	9.8749876588	6.9442891529
H49	16.5143009945	11.2198641763	8.6829968127
H50	17.3457844343	8.6688638105	5.2459522920
C51	9.9350732298	11.7184595862	5.2533656872
C52	10.1950514403	10.1449621175	3.4466694208
C53	15.2662804088	9.4216982590	6.9629389691
H54	9.6739347879	12.7128457197	5.6150025900
C55	10.2684716222	10.7238930537	6.1693520599
C56	10.5226850675	9.1465471954	4.3664013546
H57	10.1454907358	9.9045226744	2.3847314937
C58	14.3108846133	9.8571208535	7.9357894605
C59	14.7480123763	8.5004412287	6.0078355644
H60	10.2677926635	10.9536903578	7.2345594131
C61	10.5885481738	9.4316363158	5.7344394517

H62	10.7196939365	8.1337800470	4.0135858370
C63	13.0048607941	9.4512975057	7.8988975225
H64	14.5934312959	10.5259872648	8.7422765182
H65	15.3848819413	8.0680367549	5.2401629251
C66	13.4330336297	8.1217634107	6.0058574386
C67	11.0893954032	8.4014858972	6.7195970799
N68	12.5483798245	8.5952161103	6.9326862810
H69	12.2695506735	9.7705562887	8.6331955490
H70	13.0222103888	7.4219179616	5.2814008328
H71	10.6045811121	8.4899034950	7.6964564790
H72	10.9400436890	7.3789898809	6.3583772655
N73	15.2387403896	14.3403285632	7.6697163133
C74	15.4001044156	14.9564229902	9.0134026705
C75	14.0457722570	13.7755084595	7.3074342267
C76	16.3355582067	14.1064978156	6.8905991474
C77	15.8033798268	13.8950869390	10.0116064313
H78	14.4449198865	15.4236684712	9.2718152059
H79	16.1500271211	15.7491757281	8.9292446010
H80	13.1915673157	14.0333597973	7.9283934344
C81	13.9486530521	12.9477569643	6.2218941838
C82	16.2824262309	13.2965155852	5.7886872823
H83	17.2514418114	14.6003752488	7.2018726713
C84	14.8306407524	13.0648552735	10.5826800761
C85	17.1475709327	13.6670873933	10.3258421570
H86	12.9658859130	12.5464424355	5.9973584753
C87	15.0838715068	12.6206570279	5.4154810250
H88	17.2058291321	13.1755302979	5.2277372546
C89	15.1972861292	12.0037066963	11.4069773147
H90	13.7745941073	13.2556944980	10.3930075546
H91	17.9166713238	14.3337394655	9.9346369966
C92	17.5167314980	12.6008491743	11.1495350714
C93	15.0307326752	11.6641914315	4.3437411353
C94	16.5468264829	11.7430619417	11.6796229130
H95	14.4221459564	11.3807501270	11.8528986349
H96	18.5687452039	12.4418921867	11.3865083328
C97	13.8556342608	10.9182408855	4.0361694685
C98	16.1589520154	11.3541504946	3.5190899833
C99	16.9365727762	10.5072316617	12.4603675316
H100	12.9160300053	11.0847659999	4.5590741062
C101	13.8644033595	9.9224490762	3.0948353772
C102	16.1138624580	10.3622536701	2.5792136757
H103	17.0933235948	11.8998633112	3.6121996636
N104	16.9398756816	9.3329782675	11.5409870377
H105	17.9370709477	10.5867606745	12.8938646249
H106	16.2297543353	10.2863906744	13.2661496074
N107	14.9841783028	9.6118392207	2.3836931558
H108	12.9830420260	9.3276588586	2.8748361801
H109	16.9605776800	10.1193555734	1.9432469830

C110	15.7818072468	8.6601515445	11.2954350511
C111	18.0448466088	9.0597333501	10.7935304165
C112	15.0192961748	8.4389652242	1.4680445678
C113	15.6898073294	7.7526860018	10.2684962665
H114	14.9478829671	8.8751502937	11.9583575506
H115	18.9548330677	9.5866596973	11.0692568241
C116	18.0000199174	8.1559995293	9.7583600228
H117	15.3040966887	8.8035145971	0.4748620522
H118	13.9955462123	8.0589714883	1.3974861186
C119	15.9850348488	7.3795626611	1.9452534797
C120	16.7943735158	7.4935681304	9.4153125100
H121	14.7374410566	7.2469517742	10.1474724557
H122	18.9260144579	7.9856829056	9.2168695366
C123	15.6510896665	6.4769233287	2.9653731735
C124	17.2499144658	7.2976516700	1.3530455895
C125	16.6844276487	6.6269465806	8.2468544352
H126	14.6501185623	6.5018451454	3.4020196893
C127	16.5680088199	5.5074479764	3.3968260855
C128	18.1640660153	6.3336312818	1.7691979549
H129	17.5104423173	7.9811085959	0.5452683879
C130	15.4744527005	5.9862831490	7.8866087951
C131	17.7776461329	6.3987910177	7.3696507097
C132	17.8254342435	5.4441311354	2.7852579852
C133	16.2394730074	4.5385900126	4.5089297365
H134	19.1392414975	6.2685872640	1.2933851646
C135	15.3588034106	5.2863683413	6.7066841198
H136	14.5893594840	6.0337446625	8.5118496497
H137	18.7751739781	6.7681904429	7.5817409366
C138	17.6171609321	5.6927549225	6.2044032564
H139	18.5367399495	4.6794905354	3.0958652788
N140	16.4075021714	5.1711949135	5.8513039095
H141	16.9004090134	3.6656345273	4.4770785259
H142	15.2068682769	4.1807122404	4.4584243945
H143	14.4353576952	4.7994010453	6.4042289597
H144	18.4396505649	5.5184245081	5.5169254275

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N1	17.4624226323	15.8257785304	1.8911582958
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C3	16.6672522817	16.4239819442	2.8038773188
C4	16.9237651684	15.0710184132	0.9116150394
C5	19.3806709451	14.8448151912	3.0532482367
H6	19.1703292477	16.9120525740	2.3988204074
H7	19.3891103315	15.7584708494	1.0768787921
H8	17.1518651533	17.0730563073	3.5225297801
C9	15.3138893551	16.1843408186	2.8237442450
C10	15.5708591084	14.8118052049	0.8848688295
H11	17.6072042000	14.6688522010	0.1735729509

C12	19.4026242905	15.1157904562	4.4189202695
C13	19.7643035214	13.5751005048	2.6207552995
H14	14.7378357151	16.6682304530	3.6013350375
C15	14.7303134506	15.3158095397	1.8881891923
H16	15.1996609435	14.2045956101	0.0693507411
C17	19.7787694249	14.1323402953	5.3297627137
H18	19.1506486124	16.1103766471	4.7782699530
H19	19.7951120472	13.3537305881	1.5608788531
C20	20.1437398576	12.5950636778	3.5330108562
C21	13.3294673352	14.8766244353	2.0291007960
C22	20.1408346528	12.8523661870	4.9011840868
H23	19.8257173163	14.3801181627	6.3833584449
H24	20.4834381005	11.6299206952	3.1675553236
C25	12.4492878798	15.4703681417	2.9447110349
C26	12.8459336029	13.7663460831	1.3196209521
C27	20.5277475176	11.7767958078	5.8877090406
H28	12.6925862669	16.3818669393	3.4747035819
C29	11.2260319107	14.8931247418	3.2104271418
C30	11.6136329971	13.2281519130	1.6135215877
H31	13.4234291051	13.2836952529	0.5426395685
N32	19.3568704473	10.9964263628	6.3571146679
H33	21.2168185636	11.0619516829	5.4437024096
H34	21.0015251053	12.2001828208	6.7688877437
N35	10.8425881240	13.7578623492	2.5839210990
H36	10.5348133601	15.3094169513	3.9314609257
H37	11.2186691160	12.3606193525	1.0966293819
C38	18.7131494852	11.3210982062	7.5005521772
C39	18.8191277137	10.0350862353	5.5651930934
C40	9.6262931144	13.0134652208	3.0405589006
C41	17.5033455039	10.7890665067	7.8116807098
H42	19.2227171304	12.0211849542	8.1349093829
H43	19.4074833267	9.7538658848	4.7135881666
C44	17.6120524270	9.4799332058	5.8365338717
H45	8.9380653754	13.7561978664	3.4442338518
H46	9.1765283791	12.5721546632	2.1510691717
C47	10.0060542189	11.9634461091	4.0575774929
C48	16.8348364039	9.8898919331	6.9449716512
H49	17.0770573461	11.0769677274	8.7375023123
H50	17.2501479559	8.7409544676	5.1469612119
C51	10.0967978671	12.2876835035	5.4127941038
C52	10.2654998049	10.6476356884	3.6635497766
C53	15.4736533150	9.4891485575	7.1132244887
H54	9.8495859341	13.2922006687	5.7512947548
C55	10.4612090340	11.3237670111	6.3472099637
C56	10.6293029355	9.6847402203	4.5998898917
H57	10.1553043082	10.3599937671	2.6202948078
C58	14.5961184417	10.0734326677	8.0823305719
C59	14.8427608916	8.5245845022	6.2629291832

H60	10.4812395151	11.5903495639	7.4005449888
C61	10.7521405319	10.0135620690	5.9515342993
H62	10.7870883570	8.6580308753	4.2734051269
C63	13.2497356876	9.8460071182	8.0683425034
H64	14.9634320585	10.7631374750	8.8366468011
H65	15.4055061528	7.9076904414	5.5610397003
C66	13.4908390681	8.3239163125	6.2886040420
C67	11.1955055224	8.9831224675	6.9640159704
N68	12.6714424450	9.0064736865	7.1479428065
H69	12.5714414986	10.3183034198	8.7725348358
H70	12.9949421382	7.6145450265	5.6324670614
H71	10.7508619915	9.1694138104	7.9437619321
H72	10.9174606051	7.9713824061	6.6546891055
N73	15.0523165671	14.0157110872	8.0662787410
C74	15.0903987745	14.4906022098	9.4770744451
C75	13.9281710858	13.4100001511	7.5748359688
C76	16.1872087535	14.0180332402	7.3071375859
C77	15.4267370267	13.3423522326	10.4017885143
H78	14.1095546507	14.9138131041	9.7018442490
H79	15.8300589681	15.2937897533	9.5300213937
H80	13.0306548438	13.5150101263	8.1736892453
C81	13.9521887462	12.7161070725	6.3995066405
C82	16.2520579568	13.3469267788	6.1200484693
H83	17.0250066685	14.5771624452	7.7121286912
C84	14.4124081450	12.5868209053	10.9916790659
C85	16.7512585153	12.9918045769	10.6606546730
H86	13.0225885449	12.2651839043	6.0667187767
C87	15.1498972063	12.5812587297	5.6363038689
H88	17.1898213478	13.3902147392	5.5802449981
C89	14.7137961280	11.4906591213	11.7978324505
H90	13.3744285592	12.8663447699	10.8426491480
H91	17.5630219300	13.5888665072	10.2624888314
C92	17.0539124119	11.8916161489	11.4588893479
C93	15.2373146464	11.7009688961	4.5205267778
C94	16.0375327893	11.1187859055	12.0217908154
H95	13.9072135237	10.9335325314	12.2671364125
H96	18.0919566066	11.6498265484	11.6605199283
C97	14.1570727800	10.8372554873	4.1677943588
C98	16.4140729574	11.5439163518	3.7180551540
C99	16.3633843570	9.8885968922	12.8356342800
H100	13.1944602023	10.9005061946	4.6647934947
C101	14.3085639008	9.8482568474	3.2479233251
C102	16.5173763567	10.5465495547	2.7952228205
H103	17.2695856336	12.2028370444	3.8317315745
N104	16.4853601721	8.7167155474	11.9166487044
H105	17.3081050602	9.9791823505	13.3712406458
H106	15.5814351104	9.6495633446	13.5559085808
N107	15.4887122847	9.6596636455	2.5788766590

H108	13.5111950030	9.1526449104	3.0122796050
H109	17.4085208334	10.4032078420	2.1931288167
C110	15.3634610866	8.0818077750	11.5148113583
C111	17.6838955074	8.3820732220	11.3921778087
C112	15.6751741024	8.4723236925	1.7108892949
C113	15.4029487542	7.1664563824	10.4920793415
H114	14.4432940898	8.3485551938	12.0195114752
H115	18.5535831102	8.8826091412	11.7995796543
C116	17.7737688988	7.4653517765	10.3707431733
H117	16.0499840682	8.8264521045	0.7448539263
H118	14.6812816325	8.0492693121	1.5454530278
C119	16.6129259110	7.4596292583	2.3138965874
C120	16.6141267756	6.8697632008	9.8481161644
H121	14.4657023513	6.7100717757	10.2037435924
H122	18.7641215977	7.2421513709	9.9943047367
C123	16.1599936099	6.4814243282	3.2090572794
C124	17.9568375954	7.4593632976	1.9302892571
C125	16.6385137650	6.0619796246	8.6200805468
H126	15.0962021558	6.4306506268	3.4604171119
C127	17.0361064726	5.5102808987	3.7161569888
C128	18.8340094721	6.5002801120	2.4263191260
H129	18.3067456656	8.1810320795	1.1916387879
C130	15.4841058189	5.4500305706	8.1089499879
C131	17.8054389312	5.9486664747	7.8464548749
C132	18.3754662552	5.5271565634	3.3124134345
C133	16.5666097620	4.4344841881	4.6662706611
H134	19.8693429283	6.4896317077	2.0973077932
C135	15.4883516036	4.8971866102	6.8482383673
H136	14.5583037734	5.3966057430	8.6697268389
H137	18.7618171900	6.3188228937	8.1834542330
C138	17.7651413199	5.3729522202	6.6025556665
H139	19.0551752633	4.7510693721	3.6630074574
N140	16.6056203154	4.9068070416	6.0889672312
H141	17.1988941357	3.5420218262	4.6071484279
H142	15.5366286028	4.1315494282	4.4753229512
H143	14.6060172059	4.4512287618	6.4068502317
H144	18.6456525039	5.2912304044	5.9790917202

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N1	17.4983856700	15.8065193302	1.9623220653
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C3	16.6965431168	16.4010253217	2.8740491306
C4	16.9638922765	15.0611208052	0.9706007767
C5	19.4172508696	14.8101666556	3.1297994164
H6	19.2112047674	16.8832367793	2.4908589916
H7	19.4340282497	15.7387652593	1.1599559298
H8	17.1772006327	17.0449697499	3.6019563488
C9	15.3395815199	16.1654714205	2.8805298618

C10	15.6077128319	14.8064610571	0.9301240908
H11	17.6519980969	14.6632013918	0.2327202899
C12	19.4368505091	15.0702883025	4.5011947836
C13	19.8037779216	13.5425100159	2.6863863671
H14	14.7585341286	16.6464630949	3.6578578355
C15	14.7596887577	15.3053584617	1.9324009329
H16	15.2418355098	14.2071017497	0.1047742208
C17	19.8124862484	14.0793004773	5.4063696443
H18	19.1850613753	16.0622346701	4.8702631034
H19	19.8381975084	13.3298544639	1.6229130594
C20	20.1830090708	12.5540542125	3.5926946811
C21	13.3538179696	14.8669261451	2.0616857546
C22	20.1768283196	12.8019014621	4.9663612983
H23	19.8573065130	14.3197736191	6.4638735542
H24	20.5248139676	11.5918339981	3.2184213062
C25	12.4696854508	15.4565135979	2.9794671191
C26	12.8691042478	13.7619187683	1.3414381968
C27	20.5620047739	11.7186553446	5.9485129903
H28	12.7126191400	16.3638049978	3.5195528446
C29	11.2419714341	14.8801246602	3.2365693575
C30	11.6324096119	13.2237769994	1.6269478880
H31	13.4485082035	13.2814420465	0.5627896868
N32	19.3799649249	10.9403169930	6.4044218581
H33	21.2550864014	11.0059206917	5.5022823836
H34	21.0330376680	12.1355221868	6.8370151055
N35	10.8575987888	13.7494297597	2.6001488163
H36	10.5483180988	15.2940312211	3.9589223506
H37	11.2377087274	12.3604170858	1.1008760181
C38	18.7265548712	11.2625514165	7.5465720745
C39	18.8465712732	9.9850079483	5.5997366855
C40	9.6353225837	13.0056964971	3.0483616022
C41	17.5044573204	10.7304799415	7.8437943264
H42	19.2352846951	11.9588340836	8.1933974338
H43	19.4457265221	9.7047186370	4.7501054922
C44	17.6275934663	9.4301864340	5.8566038559
H45	8.9473096407	13.7482961734	3.4555498841
H46	9.1852306314	12.5724034552	2.1536756372
C47	10.0082932366	11.9487884364	4.0637223183
C48	16.8421385352	9.8387689124	6.9627428237
H49	17.0648793960	11.0181118140	8.7731205587
H50	17.2691159464	8.6945683666	5.1553055745
C51	10.0945296040	12.2676170609	5.4226490461
C52	10.2678893052	10.6326450872	3.6660218978
C53	15.4695118424	9.4396965748	7.1228464335
H54	9.8485593253	13.2716386768	5.7647410184
C55	10.4554996763	11.2995023646	6.3568547631
C56	10.6279215718	9.6647627775	4.6017561497
H57	10.1625592183	10.3485094499	2.6206401203

C58	14.5968233667	10.0187584734	8.0949018563
C59	14.8334054181	8.4882169122	6.2675480631
H60	10.4723777052	11.5629622248	7.4122065701
C61	10.7468513553	9.9888090758	5.9571234435
H62	10.7858703994	8.6386780049	4.2717497136
C63	13.2451582027	9.7969737103	8.0790290191
H64	14.9695217208	10.6992674526	8.8559055045
H65	15.3929777118	7.8784565062	5.5596214356
C66	13.4778694269	8.2899659430	6.2914698412
C67	11.1858738716	8.9512462770	6.9673639722
N68	12.6642565756	8.9687121801	7.1547678443
H69	12.5676742038	10.2654093463	8.7876823072
H70	12.9793513789	7.5870174596	5.6287159259
H71	10.7376737239	9.1314990863	7.9474914740
H72	10.9095875234	7.9405896944	6.6520329866
N73	15.0017656156	14.0616690157	8.0131653134
C74	15.0530172273	14.5407635005	9.4244077423
C75	13.8762900127	13.4522245920	7.5382020539
C76	16.1252981937	14.0666560290	7.2409587914
C77	15.4061891744	13.3945113306	10.3486948553
H78	14.0723567153	14.9616628303	9.6580330622
H79	15.7906516579	15.3469428411	9.4667888734
H80	12.9851828563	13.5574789747	8.1489760321
C81	13.8889830717	12.7531848288	6.3610263052
C82	16.1777143193	13.3895255108	6.0509597198
H83	16.9658370252	14.6318327461	7.6341181028
C84	14.4027711184	12.6322518087	10.9539016763
C85	16.7389005310	13.0544219165	10.5938802708
H86	12.9580733832	12.2958706903	6.0407490285
C87	15.0749826093	12.6189979712	5.5841545582
H88	17.1094241083	13.4342647815	5.4985800098
C89	14.7223139196	11.5401162682	11.7613293987
H90	13.3596597524	12.9049473628	10.8181707926
H91	17.5422009004	13.6594477060	10.1852198376
C92	17.0594343692	11.9586820095	11.3940230941
C93	15.1557457959	11.7240647666	4.4646882949
C94	16.0542615061	11.1787090686	11.9733894005
H95	13.9240610529	10.9788293970	12.2418332926
H96	18.1032216866	11.7261237035	11.5846851398
C97	14.0832451160	10.8491113600	4.1263679420
C98	16.3248196680	11.5691761445	3.6570705780
C99	16.4018083537	9.9562207504	12.7946482789
H100	13.1240215328	10.9048692224	4.6308993615
C101	14.2375738762	9.8482711265	3.2099765585
C102	16.4303815816	10.5599071512	2.7402077375
H103	17.1777738912	12.2338037795	3.7616230963
N104	16.5244089801	8.7706281775	11.8892704646
H105	17.3536425239	10.0597103248	13.3175931915

H106	15.6306783394	9.7168031822	13.5281946333
N107	15.4125359077	9.6632621030	2.5385789514
H108	13.4447819370	9.1431255926	2.9819124800
H109	17.3175245345	10.4169010808	2.1308211516
C110	15.4049360401	8.1146471048	11.5096791930
C111	17.7216412512	8.4422744256	11.3546731348
C112	15.6093439263	8.4660624007	1.6795331583
C113	15.4439073343	7.1832128072	10.4969443354
H114	14.4863960989	8.3762537866	12.0229416393
H115	18.5913304970	8.9587787282	11.7455220172
C116	17.8107693294	7.5105311114	10.3425263672
H117	15.9784518938	8.8158667190	0.7094979614
H118	14.6185893361	8.0326452326	1.5189215040
C119	16.5626345588	7.4644730295	2.2860423192
C120	16.6518594348	6.8931992941	9.8397944240
H121	14.5078129238	6.7101853519	10.2275469670
H122	18.8007097961	7.2942625885	9.9578404854
C123	16.1289930990	6.4811307244	3.1890449573
C124	17.9057731826	7.4840671480	1.8961637834
C125	16.6730561403	6.0749434212	8.6128553924
H126	15.0686111633	6.4203003456	3.4489554286
C127	17.0242097874	5.5255973031	3.6968260888
C128	18.8000411090	6.5401625694	2.3923349833
H129	18.2417737950	8.2092326712	1.1544670247
C130	15.5209941286	5.4445975756	8.1138258149
C131	17.8337601432	5.9775093303	7.8253324671
C132	18.3612588966	5.5634796143	3.2843230595
C133	16.5817538038	4.4420352985	4.6536113113
H134	19.8343372090	6.5443023961	2.0594482539
C135	15.5189917400	4.8886975863	6.8507959709
H136	14.5992477982	5.3822180049	8.6817580484
H137	18.7893669310	6.3666077138	8.1490119965
C138	17.7877382679	5.3992095917	6.5793254381
H139	19.0567007481	4.8009759284	3.6342141349
N140	16.6281810070	4.9152181184	6.0781661744
H141	17.2323973799	3.5628613824	4.5937603425
H142	15.5566763792	4.1162700787	4.4687640815
H143	14.6371535047	4.4283378612	6.4196418228
H144	18.6639344495	5.3296918709	5.9460896737

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N1	17.4929364144	15.5982987884	1.7828992276
C2	18.9828165669	15.5590513633	2.0069520245
C3	16.7118983206	16.3019082910	2.6371692025
C4	16.9254606505	14.8606428782	0.7966546789
C5	19.3500601469	14.4874224602	3.0229516888
H6	19.2782693688	16.5587731477	2.3414606446
H7	19.4459539488	15.3747568770	1.0329171965

H8	17.2186995205	16.9565624684	3.3434525320
C9	15.3361627939	16.1639673750	2.6146045277
C10	15.5499585559	14.7005448324	0.7292599021
H11	17.5997067051	14.3902266433	0.0840010343
C12	19.4077076301	14.7771946618	4.3958088132
C13	19.6840615203	13.1914134375	2.6011106967
H14	14.7751078869	16.7388734206	3.3460942246
C15	14.7166691851	15.2894690766	1.7009695382
H16	15.1654266518	14.0940469935	-0.0867832978
C17	19.7673300759	13.7917906678	5.3214977556
H18	19.2204094549	15.7913249741	4.7510466698
H19	19.7136194587	12.9546822947	1.5371725230
C20	20.0445860733	12.2069009465	3.5262264170
C21	13.2871495290	14.9013594089	1.8598054773
C22	20.0792893345	12.4893767810	4.8999842998
H23	19.8631575927	14.0637007277	6.3742442300
H24	20.3645733671	11.2317558578	3.1574624019
C25	12.4529782653	15.5038870374	2.8227689963
C26	12.7390034592	13.8177749966	1.1462214765
C27	20.4766040053	11.4220059447	5.9042127987
H28	12.7340373962	16.4055764638	3.3603046698
C29	11.2234255376	14.9483774781	3.1357128804
C30	11.5050293869	13.2977492284	1.4925186458
H31	13.2612883330	13.3395965898	0.3220764497
N32	19.2321058114	10.7033388908	6.4029815693
H33	21.1260717162	10.6524073494	5.4722787738
H34	20.9722854204	11.8349621356	6.7883480569
N35	10.7941209961	13.8195938897	2.5208608211
H36	10.5669561752	15.3798986193	3.8884875226
H37	11.0636058821	12.4500523255	0.9725873650
C38	18.6667072885	11.0282173231	7.5882740009
C39	18.6179575965	9.8153815630	5.5881804590
C40	9.5838288313	13.0892230325	3.0393602172
C41	17.3992907870	10.5562580308	7.9191025901
H42	19.2517379292	11.6785187643	8.2415886441
H43	19.1643916395	9.5353417546	4.6930578394
C44	17.3578254475	9.3216165704	5.8761659883
H45	8.9047052925	13.8476330637	3.4412139207
H46	9.1001881737	12.6231830423	2.1749911487
C47	9.9737549700	12.0613353195	4.0913512266
C48	16.6794012748	9.7303101261	7.0405056986
H49	16.9735290555	10.8687848289	8.8713392113
H50	16.9075080505	8.6453893821	5.1499628776
C51	10.0767944560	12.4202993807	5.4444098898
C52	10.1863387453	10.7189046862	3.7449787069
C53	15.2431926747	9.3919592882	7.2559359122
H54	9.8491135315	13.4393326441	5.7579720444
C55	10.4035030292	11.4704727328	6.4180989721

C56	10.5080173777	9.7658442971	4.7177655712
H57	10.0575440501	10.3970624834	2.7113799203
C58	14.4278099041	10.1587709087	8.1051724515
C59	14.6015538195	8.3545427770	6.5559321899
H60	10.4140564917	11.7711836406	7.4665419790
C61	10.6284404332	10.1287736866	6.0681144161
H62	10.6104930651	8.7203596857	4.4224190672
C63	13.0528324583	9.9710714098	8.1303999067
H64	14.8357345467	10.9454953858	8.7371764934
H65	15.1667747088	7.6608782560	5.9384962442
C66	13.2230340785	8.2041825466	6.6012977489
C67	10.9596078715	9.0945213668	7.1319907087
N68	12.4624520596	9.0545891714	7.3300536061
H69	12.3867179413	10.5508911916	8.7707430198
H70	12.6915976256	7.4256915831	6.0522680590
H71	10.5220270459	9.3303712226	8.1076400122
H72	10.6513582053	8.0824818686	6.8513690590
N73	15.0106623171	14.2355277014	8.0806979924
C74	15.0673918592	14.6182106947	9.5487470879
C75	13.8415948516	13.8371521918	7.5270745292
C76	16.1590670267	14.1499522891	7.3721685554
C77	15.3723628219	13.3789447955	10.3771440821
H78	14.0976619566	15.0634318635	9.7921718918
H79	15.8409237862	15.3877345687	9.6424171286
H80	12.9366790412	14.0437059128	8.1002637019
C81	13.8260566477	13.1779108361	6.3057623715
C82	16.1879256138	13.4960997993	6.1480854362
H83	17.0414232439	14.5980551328	7.8298340844
C84	14.3396880420	12.5516562355	10.8448631745
C85	16.6965330874	13.0387199003	10.6924090017
H86	12.8590833244	12.8588417681	5.9216518740
C87	15.0235965214	12.9110254239	5.6165515757
H88	17.1519948800	13.4037848506	5.6516191961
C89	14.6251055306	11.4040547217	11.5915179906
H90	13.2975712668	12.8226929739	10.6696461826
H91	17.5131706469	13.6941036661	10.3851429639
C92	16.9808110787	11.8933799181	11.4456052102
C93	15.0887296103	11.9611989802	4.4659584673
C94	15.9489923395	11.0525704536	11.8962128503
H95	13.7990462947	10.8029469721	11.9721847212
H96	18.0179888412	11.6779664336	11.7066153015
C97	14.0842603773	10.9974699362	4.2652493820
C98	16.1924929257	11.8802227912	3.5906146457
C99	16.2545634326	9.8190962143	12.7354213777
H100	13.1690674903	10.9860569888	4.8555594031
C101	14.2572748740	9.9650547925	3.3581373240
C102	16.3148624996	10.8371913741	2.6842014012
H103	16.9915619935	12.6175826540	3.6072628280

N104	16.4932784970	8.6104207487	11.8677384053
H105	17.1561071190	9.9508982307	13.3409072417
H106	15.4274208775	9.5630817739	13.4043547548
N107	15.3828563294	9.8538859411	2.6220936281
H108	13.5137185211	9.1846781057	3.2170940795
H109	17.1521614554	10.7534381232	1.9917799732
C110	15.4400983433	7.8612771948	11.4572950987
C111	17.7444803898	8.3153568082	11.4392244103
C112	15.6293404706	8.6083607747	1.7754924968
C113	15.5994019285	6.8837528443	10.4912558478
H114	14.4726754063	8.0795495251	11.9048351313
H115	18.5638984384	8.8856492583	11.8732401468
C116	17.9519473072	7.3459703009	10.4729039899
H117	15.9210877232	8.9780356519	0.7858022192
H118	14.6593450875	8.1099238016	1.6815414394
C119	16.6964083324	7.7152848211	2.3767573700
C120	16.8619731690	6.6525732235	9.9105594584
H121	14.7077952132	6.3355025730	10.1975957210
H122	18.9813854585	7.1688314553	10.1704244949
C123	16.3912069414	6.6430769953	3.2432822178
C124	18.0270024276	7.9221008028	1.9851932135
C125	17.0033310013	5.8476128413	8.6656457254
H126	15.3477087855	6.4187501695	3.4835720110
C127	17.4094905632	5.7868686650	3.7109726490
C128	19.0362047006	7.0844827836	2.4520124703
H129	18.2671345206	8.7004741332	1.2599267646
C130	15.9141888897	5.1704725360	8.0844550181
C131	18.2015108368	5.8650529064	7.9225765430
C132	18.7292033812	6.0254320937	3.3046028349
C133	17.1272510382	4.5657275320	4.5731200438
H134	20.0605418458	7.2296044630	2.1187451240
C135	15.9910842139	4.7071450960	6.7810935918
H136	14.9734891267	5.0136494836	8.6065321305
H137	19.1275477381	6.2802809543	8.3117777016
C138	18.2329292336	5.3850495447	6.6276890133
H139	19.5230340260	5.3473339411	3.6182749682
N140	17.1140783259	4.8882395481	6.0455833182
H141	17.9035811452	3.8041828629	4.4390276135
H142	16.1618981014	4.1061198430	4.3457419716
H143	15.1556553996	4.2134625915	6.2883132104
H144	19.1395144873	5.4121664065	6.0276203248

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N1	1.7995643039	5.3002038227	19.6462142156
C2	2.0265853124	4.0488907331	20.3651337692
C3	0.5320973711	5.6948283507	19.2430410869
C4	2.8088441345	6.2451507785	19.5537564330
H5	3.1026774546	3.8450846434	20.3077321188

H6	1.7832104672	4.1711677805	21.4340683008
C7	1.2391592721	2.8852576288	19.8145704092
H8	-0.2576545849	4.9678178577	19.4053641348
C9	0.3056145344	6.8833727368	18.6365450420
C10	2.6238542587	7.4488898457	18.9616201237
H11	3.7665800574	5.9373492926	19.9653934912
C12	0.0695753867	2.4891037298	20.4721218067
C13	1.6440178267	2.1862494819	18.6724906678
H14	-0.7103068407	7.0782839470	18.3094560107
C15	1.3610499186	7.8390230193	18.3661849502
H16	3.4901368643	8.1005149174	18.8957243661
C17	-0.6893421236	1.4264405957	19.9905996690
H18	-0.2433818498	3.0258979938	21.3673670875
C19	0.9015901984	1.1023009160	18.1864538099
H20	2.5577760116	2.4819141091	18.1544799711
C21	1.1921146597	8.9664441077	17.5690506721
C22	-0.2746755583	0.7415846263	18.8523503697
H23	-1.6013447072	1.1302213807	20.5042008341
C24	1.3289283428	0.3139717091	16.9667860376
C25	-0.0389448370	9.2742610467	16.8714639259
C26	2.2557507330	9.8968135401	17.2480453260
H27	-0.8633245085	-0.0947166294	18.4738118100
N28	1.3895444933	1.0683353448	15.7245836971
H29	0.6297685639	-0.5247702782	16.8336738279
H30	2.3214901139	-0.1288708731	17.1207084989
H31	-0.9099713032	8.6388323072	16.9911961099
C32	-0.1514671642	10.3002935052	15.9982108690
C33	2.1025847354	10.9162371655	16.3718504780
H34	3.2327479556	9.7915070262	17.7103535307
C35	0.2217722019	1.6294652044	15.2007946720
C36	2.5949922302	1.6312885079	15.2955817873
N37	0.8887213852	11.2003899365	15.7423304154
H38	-1.0668638443	10.4915142826	15.4444810495
H39	2.9102971388	11.6033449338	16.1318236474
C40	0.2412695551	2.6073436935	14.2645093595
H41	-0.7025916470	1.1992520289	15.5805316983
H42	3.4872861272	1.2052861267	15.7504910161
C43	2.6487678194	2.5959311191	14.3509526386
C44	0.9143366828	11.8691427536	14.4327205978
C45	1.4691363866	3.1843286766	13.7556247221
H46	-0.7202111711	2.9553234179	13.8948447084
H47	3.6356503533	2.9399390439	14.0607514691
H48	-0.0425923667	12.3910905544	14.3047918046
H49	1.7011468641	12.6322332164	14.4788839008
C50	1.1423621314	10.9115748001	13.2897734791
C51	1.5142381299	4.2406747336	12.8460494188
C52	0.0740441700	10.4690316097	12.5045559458
C53	2.4100550229	10.3635555502	13.0525767899

C54	0.3463427526	4.9503235103	12.3802462714
C55	2.7384887018	4.7489897016	12.2765624461
H56	-0.9176773251	10.8918203687	12.6664040617
C57	0.2591485985	9.4894755056	11.5304816566
C58	2.5918858059	9.3803277303	12.0860012417
H59	3.2589753681	10.7030870567	13.6457006658
C60	0.4235647780	6.0105325875	11.5434681713
H61	-0.6449582869	4.6771535904	12.7301413691
H62	3.6818495872	4.2568386621	12.4842766160
C63	2.7726438388	5.8008568516	11.4236436009
H64	-0.5882871928	9.1551109004	10.9310879647
C65	1.5157790501	8.9162967600	11.3187367407
H66	3.5810150874	8.9511830098	11.9312552102
N67	1.6229994358	6.4596632502	11.0130050833
H68	-0.4542046843	6.5747489093	11.2359974660
H69	3.6975027985	6.1634007032	10.9798054589
C70	1.6811452848	7.7626455012	10.3588785509
H71	2.6420554798	7.8201673237	9.8346109817
H72	0.8906448789	7.7959274359	9.5958538741
N73	5.6553763185	1.3536051047	11.4168052493
C74	6.8108941567	1.6569156607	12.2775979141
C75	4.5279620102	0.7852465667	12.0293100490
C76	5.3820586429	2.2304804820	10.3595457293
C77	6.5308061601	2.7418900077	13.2885542355
H78	7.6371702272	1.9372196144	11.6117641729
H79	7.1004265183	0.7296759028	12.7877393159
H80	4.7494132103	0.1369173360	12.8738862013
C81	3.2640511948	1.0146354290	11.6108387957
C82	4.1303486214	2.4887105055	9.9168088138
H83	6.2640645136	2.6645662318	9.8931995929
C84	6.3313418090	2.4386895503	14.6389575267
C85	6.3733917633	4.0739688925	12.8811048103
H86	2.4697075126	0.5160592480	12.1596964779
C87	2.9439405965	1.9278469319	10.5336827651
H88	4.0418519529	3.1495880486	9.0596748225
C89	5.9662894796	3.4300478318	15.5502520171
H90	6.4542826248	1.4097313432	14.9781147554
H91	6.5286282342	4.3361275356	11.8350950455
C92	5.9994965025	5.0591126320	13.7887344688
C93	1.6455298012	2.3053402687	10.2018838424
C94	5.7802241543	4.7519949284	15.1366194993
H95	5.8098573238	3.1712189490	16.5982081208
H96	5.8559907119	6.0833879731	13.4451054891
C97	0.4661272422	1.8112220680	10.8830500588
C98	1.3332599808	3.3103247418	9.2073267154
C99	5.2707094406	5.8053810448	16.0913648397
H100	0.5513835519	1.0538643622	11.6558628380
C101	-0.7733385864	2.3123326878	10.6564636241

C102	0.0773799935	3.7824898805	9.0161643921
H103	2.1221843953	3.7627076015	8.6137043974
N104	3.8379153228	6.0340358952	15.9755813178
H105	5.7699571896	6.7658373958	15.9168465655
H106	5.4858713530	5.5113070124	17.1286945239
N107	-1.0040673515	3.3376876012	9.7538981892
H108	-1.6450204399	1.9664188679	11.2031726882
H109	-0.1470767860	4.5667366819	8.2977404946
C110	2.9484281966	5.0857286870	16.4483868138
C111	3.3159544916	7.0516135353	15.1973325614
C112	-2.3459229628	3.8328323886	9.4465240697
C113	1.6196552673	5.1551540467	16.2154756739
H114	3.3978368307	4.2756930391	17.0162018747
H115	4.0404169373	7.7761607921	14.8340795600
C116	1.9904729891	7.1576380242	14.9400011864
H117	-2.7955409175	3.2227765841	8.6453608308
H118	-2.2218081168	4.8446888058	9.0401266252
C119	-3.2880704368	3.8537664470	10.6249282436
C120	1.0206901101	6.2116198082	15.4347646811
H121	1.0118001902	4.3541149079	16.6234564856
H122	1.6749064036	8.0182756468	14.3604393491
C123	-4.1827283540	2.7901879827	10.7905106707
C124	-3.3197198021	4.9152460848	11.5372534055
C125	-0.3422198867	6.2937280293	15.1521636714
H126	-4.1717393416	1.9699089227	10.0724943028
C127	-5.0788114947	2.7773451702	11.8554981619
C128	-4.2347796683	4.9297847038	12.5992851703
H129	-2.6315611249	5.7518814700	11.4112457181
C130	-1.3299619794	5.3375722232	15.6100016673
C131	-0.9106578008	7.3068555179	14.2869375601
H132	-5.7663272717	1.9434392972	11.9806266991
C133	-5.0998315186	3.8413353566	12.7534318670
C134	-4.3280344583	6.0830069545	13.5779522105
C135	-2.6214701295	5.3639538030	15.2044932490
H136	-1.0429610638	4.5421713772	16.2942781140
H137	-0.2905392143	8.1124310297	13.9107802999
C138	-2.2031860370	7.3037403403	13.8968403784
H139	-5.8078172807	3.8413665309	13.5826450637
N140	-3.1272248629	6.3563895933	14.3545637991
H141	-5.1565720699	5.8795727281	14.2731586909
H142	-4.5823560446	7.0132540935	13.0524905624
H143	-3.3556473961	4.6336486550	15.5381454929
H144	-2.6187781932	8.0619893326	13.2352756789

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N1	1.4897149008	5.2692527327	19.7299120375
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C4	2.4677648538	6.2489044918	19.6585250831
H5	2.7912798215	3.9096025141	20.5736392879
H6	1.3070025756	4.1266885888	21.4986109384
C7	1.0923437659	2.8200061342	19.8190858529
H8	-0.5356856436	4.8463012345	19.3869913517
C9	-0.0062657902	6.7652559650	18.5964769790
C10	2.2682572317	7.4283562123	19.0214326758
H11	3.4118554757	5.9941233153	20.1326704726
C12	-0.0285104788	2.2179582737	20.3997624823
C13	1.6107733736	2.2780347369	18.6395828763
H14	-1.0140913212	6.9132344845	18.2229495358
C15	1.0207461885	7.7600749745	18.3637591577
H16	3.1078112107	8.1161565865	18.9922378672
C17	-0.6192827671	1.1024135925	19.8131261113
H18	-0.4377008032	2.6333544769	21.3192995808
C19	1.0320348689	1.1533926232	18.0424315648
H20	2.4878971268	2.7355442703	18.1791338916
C21	0.8376525886	8.8779075872	17.5500813393
C22	-0.0924058160	0.5753572660	18.6379767810
H23	-1.4936337652	0.6451895293	20.2702392571
C24	1.6006004665	0.5467364563	16.7796813902
C25	-0.4000309004	9.1706962885	16.8580306272
C26	1.8823520320	9.8327747839	17.2418560963
H27	-0.5518221448	-0.2972459521	18.1750651875
N28	1.6243413777	1.4657810609	15.6469540636
H29	1.0154727155	-0.3404350938	16.5047852348
H30	2.6301732805	0.2062361746	16.9398591885
H31	-1.2693403115	8.5345309335	16.9921966047
C32	-0.5320930736	10.2010199056	15.9919583889
C33	1.7116659587	10.8512877278	16.3654218641
H34	2.8587168599	9.7481318591	17.7086813294
C35	0.4426028251	1.8974538212	15.0732214112
C36	2.7997563180	2.0232221300	15.1922989638
N37	0.4975110553	11.1046212913	15.7304414532
H38	-1.4561782871	10.3924885301	15.4524847608
H39	2.5048973259	11.5569761880	16.1319872499
C40	0.4239570357	2.8388997982	14.0936843837
H41	-0.4588676105	1.4265823160	15.4548345281
H42	3.7048142903	1.6503700215	15.6624386401
C43	2.8217416402	2.9664958097	14.2160633695
C44	0.4937155081	11.8184771178	14.4468665864
C45	1.6237970916	3.4681499397	13.6036012064
H46	-0.5464864093	3.1083182615	13.6890497133
H47	3.7974164803	3.3339571142	13.9170231536
H48	-0.4879659644	12.2933615617	14.3279637353
H49	1.2390982518	12.6194949615	14.5222469617
C50	0.7838676465	10.9146449274	13.2726489157
C51	1.6221426892	4.5005178123	12.6453903989

C52	-0.2304319886	10.5181108045	12.3958130274
C53	2.0694366707	10.3899021059	13.0800809552
C54	0.4215927491	5.0443770931	12.0803991517
C55	2.8203755731	5.1191672279	12.1442366438
H56	-1.2352315054	10.9219934814	12.5231010025
C57	0.0267357670	9.6127457198	11.3659254194
C58	2.3243917903	9.4832847665	12.0575660902
H59	2.8786357270	10.6914121445	13.7443059433
C60	0.4359607234	6.0862521081	11.2125134848
H61	-0.5498851747	4.6419678209	12.3501124203
H62	3.7969588983	4.7576163863	12.4484205431
C63	2.7918890441	6.1569229235	11.2679458937
H64	-0.7774591969	9.3182499075	10.6910706132
C65	1.3048963089	9.0745633332	11.1880347048
H66	3.3298375776	9.0812160701	11.9321890099
N67	1.6077769355	6.6655395141	10.7687092953
H68	-0.4727859506	6.5183977433	10.8003052950
H69	3.6943139253	6.6296770656	10.8889315333
C70	1.5653368227	8.0016767641	10.1596895260
H71	2.5233037970	8.1556127833	9.6500999840
H72	0.7805453780	7.9993124123	9.3933226812
N73	5.4462950748	1.1897735763	11.5477319226
C74	6.6618127736	1.3742264217	12.3530557211
C75	4.3261186145	0.6165785192	12.1509833988
C76	5.1918784329	2.0845645738	10.5093500251
C77	6.5241226222	2.4746899647	13.3764965230
H78	7.4791255954	1.5871912729	11.6539944933
H79	6.8881411911	0.4197014296	12.8434415972
H80	4.5477008826	-0.0651120629	12.9683920165
C81	3.0621828828	0.8696014810	11.7407790990
C82	3.9417939986	2.3639690556	10.0705753398
H83	6.0786359954	2.5157509430	10.0516903446
C84	6.3526653534	2.1858735156	14.7336410334
C85	6.4889558247	3.8179020933	12.9748947882
H86	2.2652416629	0.3526177249	12.2668125668
C87	2.7530014792	1.8054634368	10.6806301872
H88	3.8599767274	3.0456691783	9.2299408585
C89	6.1348085380	3.2048095117	15.6607512882
H90	6.3912519344	1.1489326562	15.0686275005
H91	6.6405998733	4.0698192042	11.9259345411
C92	6.2620994210	4.8327700428	13.8979328894
C93	1.4552826601	2.1723862306	10.3228496144
C94	6.0723500915	4.5411809025	15.2553855071
H95	6.0091306591	2.9576770041	16.7156241848
H96	6.2307188196	5.8691412410	13.5618771557
C97	0.2698863734	1.6832321543	10.9950170485
C98	1.1475037186	3.1277202883	9.2785075626
C99	5.7098026444	5.6334891307	16.2310110470

H100	0.3443260295	0.9289930679	11.7709864342
C101	-0.9702678224	2.1651896094	10.7337684233
C102	-0.1093037913	3.5776490619	9.0468287576
H103	1.9363874164	3.5381972365	8.6551388577
N104	4.2851774226	5.9810234466	16.1547986658
H105	6.2787102209	6.5499426864	16.0383547251
H106	5.9266034151	5.3218585419	17.2604700852
N107	-1.1955580744	3.1623038952	9.7974145357
H108	-1.8504613060	1.8142569909	11.2643121480
H109	-0.3335197125	4.3088253730	8.2745645001
C110	3.3438853296	5.1022247603	16.6480034564
C111	3.8395742531	6.9758701691	15.3066720840
C112	-2.5452082853	3.6338925150	9.4873100856
C113	2.0236540932	5.2046524283	16.3551971378
H114	3.7394590481	4.3279809782	17.3001981589
H115	4.6070609894	7.6527356144	14.9395668296
C116	2.5268737986	7.1131546349	14.9863055996
H117	-3.0497155971	2.9256820205	8.8102809642
H118	-2.4302752877	4.5739999780	8.9337548334
C119	-3.4045186898	3.8405636111	10.7121335579
C120	1.5147335883	6.2152162652	15.4731084448
H121	1.3605485754	4.4691738504	16.8008094396
H122	2.2598414103	7.9505882935	14.3501797861
C123	-4.3966962251	2.9013878422	11.0185508344
C124	-3.2385922945	4.9438126789	11.5560961104
C125	0.1590769223	6.3125288706	15.1044416560
H126	-4.5354688970	2.0414930493	10.3634982096
C127	-5.1981110561	3.0572260161	12.1458796034
C128	-4.0418444058	5.1181928872	12.6888447935
H129	-2.4765113649	5.6906730317	11.3237673059
C130	-0.8664080616	5.4218327678	15.5871877771
C131	-0.3294577942	7.2945122081	14.1747358310
H132	-5.9629028000	2.3183165557	12.3769585519
C133	-5.0178723304	4.1591970508	12.9785006077
C134	-3.8793709898	6.3179996016	13.5973615949
C135	-2.1485068027	5.4776707607	15.1406535070
H136	-0.6352349386	4.6681358845	16.3339799904
H137	0.3310325103	8.0518151411	13.7670844238
C138	-1.6179649957	7.3194572592	13.7507915734
H139	-5.6433869955	4.2847276806	13.8617657548
N140	-2.5589839191	6.4181244211	14.2101055133
H141	-4.6350717111	6.2777543296	14.3931259773
H142	-4.0496764792	7.2516434173	13.0469610607
H143	-2.9241310161	4.8022220801	15.4915116121
H144	-1.9833902364	8.0528259259	13.0366509416

mHo²⁺ -3218.22289994678

N1	0.9765276038	5.1897125186	19.8477604968
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C2	1.1266326200	3.9151745490	20.5532374417
C3	-0.2566918705	5.5704646038	19.3507584062
C4	2.0391284836	6.0451070628	19.6516875432
H5	2.1793726821	3.8319686885	20.8424893022
H6	0.5393870166	3.9445589353	21.4813304819
C7	0.6945543373	2.7274858743	19.7226551622
H8	-1.0797959445	4.8989719244	19.5773883485
C9	-0.4216716876	6.7086949451	18.6290447386
C10	1.9164794489	7.1928824045	18.9347918318
H11	2.9776357837	5.7329325481	20.1014060847
C12	-0.4746664576	2.0404922185	20.0633183639
C13	1.4309180268	2.2984288340	18.6130484897
H14	-1.4266604066	6.9256350055	18.2810752211
C15	0.6766060904	7.5910046507	18.3150962195
H16	2.8139317830	7.7917287354	18.8202314277
C17	-0.9009819403	0.9491244614	19.3118041187
H18	-1.0503433478	2.3656891763	20.9293547544
C19	1.0133191292	1.2027756772	17.8494100264
H20	2.3570040207	2.8149134739	18.3526675269
C21	0.5576496259	8.7096974516	17.4708078212
C22	-0.1612261875	0.5349827875	18.2076123222
H23	-1.8113429090	0.4214371255	19.5857586580
C24	1.8021535035	0.7205932339	16.6542644458
C25	-0.6733987081	9.0985594501	16.8282878625
C26	1.6669505555	9.5720330545	17.1418620127
H27	-0.4902800197	-0.3194535200	17.6173892763
N28	1.8119335760	1.6826511079	15.5440670763
H29	1.3867788864	-0.2285963727	16.2927566106
H30	2.8477271558	0.5307420821	16.9200263470
H31	-1.5930600880	8.5516270335	17.0150896975
C32	-0.7430263025	10.1369366436	15.9553413569
C33	1.5522827172	10.6057049058	16.2701355368
H34	2.6421093182	9.4179128669	17.5926373647
C35	0.6322024104	2.0640290801	14.9450648401
C36	2.9734688332	2.2608785913	15.1072240372
N37	0.3522301233	10.9305374110	15.6600260321
H38	-1.6665426392	10.4184224668	15.4560845705
H39	2.3871419443	11.2572013616	16.0267228444
C40	0.6021138787	3.0037004713	13.9602864992
H41	-0.2615669403	1.5664266118	15.3101396937
H42	3.8797924744	1.9202115857	15.5973021109
C43	2.9898091997	3.2004593767	14.1199326032
C44	0.3562961325	11.7607013659	14.4457630005
C45	1.7910977787	3.6595678351	13.4890806355
H46	-0.3706870239	3.2428645034	13.5444740448
H47	3.9627593073	3.5964774862	13.8413852635
H48	-0.6319998643	12.2246789709	14.3545984404
H49	1.0874120550	12.5625431384	14.6020948845

C50	0.6907070319	10.9474468364	13.2193361022
C51	1.7789397580	4.6833807804	12.5072041814
C52	-0.3078554142	10.5022350040	12.3477162708
C53	2.0125446932	10.5458260802	12.9779080900
C54	0.5767953333	5.1512312659	11.8931376896
C55	2.9638901250	5.3543507163	12.0467519976
H56	-1.3377507873	10.8240775764	12.5035704838
C57	-0.0018946041	9.6517358221	11.2850555871
C58	2.3168614032	9.6933742858	11.9225663521
H59	2.8125152313	10.9077918485	13.6230403076
C60	0.5645782813	6.1949021753	11.0199187626
H61	-0.3756388003	4.6779764988	12.1111941119
H62	3.9483445399	5.0434232602	12.3842093673
C63	2.9087679170	6.3947149176	11.1695813466
H64	-0.7940766113	9.3170988885	10.6146205015
C65	1.3108089141	9.2207371845	11.0691425494
H66	3.3504449663	9.3914158664	11.7543753440
N67	1.7172460283	6.8426882841	10.6424712453
H68	-0.3473252783	6.5636961738	10.5558509675
H69	3.7963919160	6.9164138906	10.8213884056
C70	1.6278218050	8.1803987805	10.0245302245
H71	2.5859152584	8.3752688827	9.5312211748
H72	0.8534680981	8.1424861933	9.2500584928
N73	5.3195549249	1.2380010588	11.6230787702
C74	6.6218290969	1.3266627992	12.3021171714
C75	4.2567850357	0.6094903973	12.2479761521
C76	5.0188452365	2.1303068958	10.6074644430
C77	6.6235205585	2.4221169910	13.3397948692
H78	7.3790121942	1.5047110123	11.5301417631
H79	6.8312535431	0.3512479927	12.7556666586
H80	4.5294826013	-0.0860273515	13.0376405303
C81	2.9674408892	0.8254892592	11.8797300945
C82	3.7441258093	2.3804498292	10.2145825902
H83	5.8767751356	2.5926233658	10.1271236459
C84	6.4676590066	2.1326408095	14.6981590249
C85	6.6864706475	3.7676075902	12.9478367930
H86	2.2062459291	0.2622890305	12.4102820487
C87	2.6035019452	1.7664290251	10.8502874128
H88	3.6148359395	3.0716729395	9.3882714615
C89	6.3397124733	3.1571547481	15.6362045658
H90	6.4452195149	1.0926477419	15.0251422352
H91	6.8431438665	4.0170043054	11.8991005959
C92	6.5524681241	4.7887806443	13.8817834597
C93	1.2734708647	2.0765946550	10.5129791438
C94	6.3591015425	4.4978053472	15.2387196473
H95	6.2220829456	2.9116604165	16.6919495301
H96	6.6008595744	5.8276285692	13.5555314430
C97	0.1290275530	1.5069943128	11.1816682372

C98	0.9154981639	3.0204820698	9.4829755342
C99	6.0636191170	5.6031921578	16.2205466054
H100	0.2490388543	0.7386114540	11.9370983124
C101	-1.1407469850	1.9112600359	10.9170268515
C102	-0.3695985336	3.3938672532	9.2479675749
H103	1.6765460527	3.4902512882	8.8690687573
N104	4.6427010731	5.9964342669	16.1453458079
H105	6.6590741934	6.4995873243	16.0180978150
H106	6.2711277505	5.2886768784	17.2496024597
N107	-1.4220711974	2.8884833302	9.9794059055
H108	-2.0008136509	1.4941244140	11.4311030668
H109	-0.6374279493	4.1157233595	8.4814350256
C110	3.6841488603	5.1783101766	16.6943687144
C111	4.2293895309	6.9681154068	15.2606470392
C112	-2.8014913358	3.3284325079	9.7457367014
C113	2.3634429139	5.3105037113	16.3931290778
H114	4.0555061393	4.4366481392	17.3972284135
H115	5.0182127203	7.6014311129	14.8635224440
C116	2.9184859048	7.1329624565	14.9317039021
H117	-3.3575683018	2.5322046154	9.2310448875
H118	-2.7504636501	4.1805988829	9.0586996375
C119	-3.5193764748	3.7017329949	11.0224726526
C120	1.8874178436	6.2800537256	15.4569443003
H121	1.6731383058	4.6393016555	16.8958831060
H122	2.6775943853	7.9454926245	14.2526520156
C123	-4.5030129773	2.8488434624	11.5324908187
C124	-3.2158350701	4.8752114736	11.7212527982
C125	0.5250985087	6.3776914006	15.0736677393
H126	-4.7500941923	1.9368679836	10.9902726191
C127	-5.1633291116	3.1570860373	12.7186014563
C128	-3.8711300037	5.1959634169	12.9153551236
H129	-2.4701913613	5.5607005744	11.3148814420
C130	-0.5045593074	5.5214351293	15.5945580572
C131	0.0511311226	7.3288180926	14.1155755669
H132	-5.9249998247	2.4861152672	13.1075763647
C133	-4.8437647800	4.3227912314	13.4090908549
C134	-3.5580852276	6.4634570041	13.6774811362
C135	-1.7940940606	5.5913297671	15.1646477656
H136	-0.2850427354	4.7856357079	16.3607212779
H137	0.7186707240	8.0555665270	13.6629499332
C138	-1.2476926062	7.3577105580	13.7049183135
H139	-5.3571699039	4.5662441530	14.3385631378
N140	-2.1887049341	6.4971233743	14.2050366973
H141	-4.2559689160	6.5743527334	14.5161815556
H142	-3.6792875587	7.3481035064	13.0428889958
H143	-2.5787384863	4.9477945584	15.5519960155
H144	-1.6055296223	8.0655788903	12.9639548392

mHo³⁺ -3218.09613513569

N1	0.9396915287	5.2372865045	19.8975137709
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C4	2.0265632707	6.0423273935	19.6781074833
H5	2.1048021010	3.8615844182	20.9254548182
H6	0.4540129532	4.0137143969	21.5303216018
C7	0.6186796996	2.7801779004	19.7768612888
H8	-1.1198076754	4.9901045205	19.6341823633
C9	-0.4129542311	6.7625815804	18.6447335870
C10	1.9355089782	7.1822447294	18.9334167751
H11	2.9569133521	5.7127703928	20.1317977309
C12	-0.5849164711	2.1349009990	20.0780949427
C13	1.3815147069	2.3211426994	18.6964763508
H14	-1.4124970728	7.0025428992	18.2972066154
C15	0.7086631417	7.5974034100	18.3224331877
H16	2.8490293150	7.7529713743	18.8069920094
C17	-1.0196283644	1.0547772472	19.3151723753
H18	-1.1789298980	2.4802825871	20.9234144261
C19	0.9531930045	1.2377626287	17.9197367358
H20	2.3388414077	2.7980634633	18.4757909702
C21	0.6173495265	8.7233353594	17.4557710809
C22	-0.2557842473	0.6114585796	18.2389741910
H23	-1.9542217695	0.5562985153	19.5603750151
C24	1.7665750440	0.7212277245	16.7554369226
C25	-0.6047596335	9.1354756533	16.8324931873
C26	1.7476827658	9.5397035887	17.1189664237
H27	-0.5916906323	-0.2370999542	17.6438823656
N28	1.7793635639	1.6454076202	15.6064679101
H29	1.3668181586	-0.2428040525	16.4181463534
H30	2.8104933859	0.5544637874	17.0405251875
H31	-1.5419842931	8.6321447011	17.0467993422
C32	-0.6487964880	10.1623527078	15.9365181528
C33	1.6583523396	10.5625156132	16.2244938358
H34	2.7183402977	9.3711000806	17.5714254426
C35	0.6034325438	1.9936484073	14.9853098312
C36	2.9391580768	2.2150158946	15.1577205429
N37	0.4710530827	10.8906696926	15.6121381967
H38	-1.5686897766	10.4713453701	15.4475130328
H39	2.5100373531	11.1851349942	15.9658414481
C40	0.5701456710	2.9189632554	13.9850951188
H41	-0.2862049928	1.4841898541	15.3441946787
H42	3.8464617436	1.8891890656	15.6563415491
C43	2.9533527634	3.1369486702	14.1511227361
C44	0.4744580354	11.7504483858	14.4118847280
C45	1.7525134095	3.5879562116	13.5197080460
H46	-0.3992621371	3.1328054966	13.5492083987
H47	3.9258175981	3.5324749509	13.8709931425

H48	-0.5021707539	12.2398595305	14.3501898252
H49	1.2318231950	12.5262591517	14.5673179916
C50	0.7625544230	10.9259341446	13.1804931682
C51	1.7297028737	4.6191096885	12.5391048297
C52	-0.2679030312	10.4837897826	12.3457446157
C53	2.0719875676	10.5061614916	12.9082688500
C54	0.5226650456	5.0948629923	11.9423861690
C55	2.9105879801	5.2898655651	12.0723750091
H56	-1.2884970891	10.8224450382	12.5244958165
C57	-0.0032258012	9.6119086448	11.2883243556
C58	2.3349538314	9.6333853756	11.8582562835
H59	2.8952913462	10.8694920245	13.5225994819
C60	0.5088071382	6.1354548116	11.0623553766
H61	-0.4333402293	4.6375363458	12.1802408621
H62	3.8950968838	4.9827382188	12.4097174358
C63	2.8531204506	6.3235058659	11.1859273101
H64	-0.8184324001	9.2793356964	10.6449519294
C65	1.2969447898	9.1584029484	11.0456875383
H66	3.3600140910	9.3191527120	11.6626567484
N67	1.6594184291	6.7709831458	10.6692532606
H68	-0.4062857850	6.5139290975	10.6125705854
H69	3.7401390503	6.8381542789	10.8263652769
C70	1.5730745999	8.0926799342	10.0143342217
H71	2.5210577316	8.2612564580	9.4931455814
H72	0.7792328162	8.0442397556	9.2610990225
N73	5.3212467575	1.4114771383	11.5482630803
C74	6.6461610429	1.4374024462	12.2008452102
C75	4.2896106244	0.7075932628	12.1212739519
C76	5.0167626185	2.3416441401	10.5814290309
C77	6.6577239503	2.4864611524	13.2862884790
H78	7.3895868355	1.6450065996	11.4244649841
H79	6.8433225848	0.4364107845	12.5979629892
H80	4.5788470812	-0.0288232577	12.8662222075
C81	2.9925089816	0.9095730975	11.7535758268
C82	3.7333603706	2.5866415236	10.1939134440
H83	5.8659224871	2.8508674455	10.1351151487
C84	6.4652790636	2.1472970408	14.6286523610
C85	6.7527904261	3.8426393139	12.9447039074
H86	2.2442730687	0.2890294579	12.2360201947
C87	2.6233626721	1.8967082614	10.7844906988
H88	3.5900112842	3.3174328006	9.4063334783
C89	6.3273381255	3.1399517653	15.6002169798
H90	6.4215745832	1.0970674665	14.9177505719
H91	6.9454346818	4.1277930773	11.9110217561
C92	6.6053478027	4.8314493378	13.9111094375
C93	1.2705370607	2.1789772519	10.4439651192
C94	6.3685923422	4.4932706500	15.2497020524
H95	6.1848587425	2.8577413044	16.6437565687

H96	6.6797124054	5.8800015760	13.6240444995
C97	0.1571664958	1.5301725236	11.0746737169
C98	0.9033441283	3.1504268946	9.4579642252
C99	6.0595416353	5.5707990329	16.2593635632
H100	0.3000737315	0.7329397023	11.7952926036
C101	-1.1290642223	1.8871807152	10.8025490607
C102	-0.4018014056	3.4720173818	9.2150107239
H103	1.6527559172	3.6774734480	8.8765142607
N104	4.6352489653	5.9581866944	16.1737366267
H105	6.6539600899	6.4737693681	16.0882455955
H106	6.2509736378	5.2310932061	17.2820330039
N107	-1.4315599620	2.8784325365	9.8973041672
H108	-1.9772213682	1.4090331668	11.2828011568
H109	-0.6921728319	4.2125849368	8.4751363520
C110	3.6790899715	5.1445575277	16.7266516227
C111	4.2252864740	6.9434641645	15.3072084349
C112	-2.8327521354	3.2999179376	9.7018306710
C113	2.3559914664	5.2849863374	16.4307648810
H114	4.0508496164	4.3959680632	17.4220033105
H115	5.0152268027	7.5784125457	14.9150059379
C116	2.9122016430	7.1165957661	14.9828794861
H117	-3.3741583385	2.4896497389	9.1977280115
H118	-2.8129596177	4.1553869800	9.0185985643
C119	-3.5133300554	3.6456570733	11.0061376550
C120	1.8813594203	6.2618774263	15.5037311009
H121	1.6662355017	4.6089662426	16.9270145620
H122	2.6740344075	7.9343340340	14.3089446190
C123	-4.4372317493	2.7517062945	11.5579985396
C124	-3.2297462090	4.8333739359	11.6908443496
C125	0.5144338630	6.3612591016	15.1195432624
H126	-4.6722608016	1.8298913955	11.0269618798
C127	-5.0574000283	3.0340903348	12.7718955304
C128	-3.8442568953	5.1269997223	12.9142502632
H129	-2.5380463928	5.5533521227	11.2488235522
C130	-0.5150425581	5.5001737263	15.6303361556
C131	0.0433904770	7.3140215417	14.1635165697
H132	-5.7755162492	2.3338342721	13.1914709520
C133	-4.7575400478	4.2132033924	13.4490033301
C134	-3.5535048996	6.4076147461	13.6634204997
C135	-1.8010150892	5.5593431636	15.1830132094
H136	-0.2986949585	4.7667227506	16.3988783307
H137	0.7097646414	8.0476077366	13.7198605044
C138	-1.2522949084	7.3308593210	13.7354244183
H139	-5.2444030206	4.4363297835	14.3977495506
N140	-2.1880035828	6.4561161192	14.2146269457
H141	-4.2617074326	6.5264065516	14.4919215919
H142	-3.6666304037	7.2833446111	13.0157997948
H143	-2.5863064844	4.9126425987	15.5636484892

H144 -1.6065609689 8.0372580457 12.9910536612

mHo⁴⁺ -3217.95515941433

N1	0.9617434701	5.3106804850	19.9550200214
C2	1.0893324820	3.9965833830	20.6348753863
C3	-0.2574508708	5.7214116175	19.4850893709
C4	2.0541800087	6.0905126919	19.7136955393
H5	2.1447792467	3.8786949109	20.8987325397
H6	0.5170880098	4.0429312345	21.5684972612
C7	0.5929419269	2.8656437094	19.7631050114
H8	-1.1064180472	5.0988810734	19.7509681485
C9	-0.3917914619	6.8550955792	18.7337724802
C10	1.9658387808	7.2372517567	18.9675230679
H11	2.9871531200	5.7514867384	20.1553016703
C12	-0.6807902599	2.3339905677	19.9945382565
C13	1.3655989991	2.3441736276	18.7167542387
H14	-1.3967521634	7.1161164633	18.4184818863
C15	0.7358896149	7.6588730592	18.3882632997
H16	2.8846436366	7.7984546567	18.8274457693
C17	-1.1762738702	1.3091606510	19.1935176592
H18	-1.2803620009	2.7185132141	20.8189993038
C19	0.8746974591	1.3148334395	17.9014918755
H20	2.3784655481	2.7212994840	18.5589866949
C21	0.6399749674	8.7945690509	17.5062942386
C22	-0.4037247321	0.8050554452	18.1506896416
H23	-2.1635937468	0.8974711394	19.3867251050
C24	1.6879934351	0.7350844551	16.7670088761
C25	-0.5863871966	9.1979904512	16.9054559089
C26	1.7672040777	9.5972476917	17.1616280385
H27	-0.7858243330	-0.0075306269	17.5334596554
N28	1.7189383781	1.6168332739	15.5767559733
H29	1.2743727947	-0.2315990945	16.4578845509
H30	2.7284151893	0.5645512204	17.0612695119
H31	-1.5241099371	8.7075942552	17.1450834561
C32	-0.6378324994	10.2188767708	15.9949376012
C33	1.6684844174	10.6159321722	16.2545876028
H34	2.7393890963	9.4379784375	17.6133729073
C35	0.5582843155	1.9272297634	14.9142625652
C36	2.8815421275	2.1878393856	15.1470486114
N37	0.4810668245	10.9232992257	15.6489267427
H38	-1.5636693091	10.5322317743	15.5199630260
H39	2.5174273950	11.2375639490	15.9841441787
C40	0.5336378135	2.8445306653	13.9027115958
H41	-0.3293397027	1.3970542780	15.2472117758
H42	3.7810745160	1.8807266930	15.6716300787
C43	2.9085849104	3.0977216527	14.1263643176
C44	0.4652172186	11.7966612967	14.4494420015
C45	1.7167356626	3.5320386940	13.4718093703

H46	-0.4295479970	3.0309422696	13.4365887197
H47	3.8817322131	3.5042362223	13.8656753388
H48	-0.5151852831	12.2802017890	14.4017556585
H49	1.2218545994	12.5728878075	14.6009810093
C50	0.7480764634	10.9602110223	13.2228971302
C51	1.7075156941	4.5811743393	12.4989215911
C52	-0.2874053495	10.4926797576	12.4081997632
C53	2.0607673723	10.5616527381	12.9366596831
C54	0.5067549745	5.0638974415	11.9009716556
C55	2.8923718102	5.2639423475	12.0655878203
H56	-1.3106866882	10.8188829542	12.5942474275
C57	-0.0218695873	9.6144913560	11.3550224623
C58	2.3241775959	9.6810845928	11.8918841359
H59	2.8876520132	10.9501613522	13.5306220453
C60	0.4999582541	6.1345054443	11.0517696772
H61	-0.4532883935	4.6001721255	12.1153671179
H62	3.8765525027	4.9522514719	12.4042759282
C63	2.8395619004	6.3280975773	11.2098978846
H64	-0.8400235916	9.2691104177	10.7220684906
C65	1.2827647246	9.1793964454	11.1003706543
H66	3.3527935903	9.3889121749	11.6816871781
N67	1.6495395786	6.7901633369	10.7065670022
H68	-0.4108784085	6.5225998362	10.6006297327
H69	3.7283682735	6.8556316233	10.8730760962
C70	1.5653867564	8.1218927107	10.0600853572
H71	2.5160569173	8.2945025471	9.5459925764
H72	0.7758089891	8.0755934818	9.3028836839
N73	5.3317981071	1.4364927837	11.5192643867
C74	6.6590943956	1.4553657085	12.1807908286
C75	4.3128093062	0.6978971783	12.0534003613
C76	5.0458633308	2.3493331288	10.5416352199
C77	6.6448802436	2.4858610299	13.2862134348
H78	7.4030761082	1.6872176031	11.4119222790
H79	6.8597016067	0.4474746794	12.5565348216
H80	4.5991709073	-0.0419678494	12.7961343734
C81	3.0159368206	0.8732240708	11.6515304549
C82	3.7639420558	2.5698877545	10.1206645325
H83	5.8958988603	2.8728656454	10.1137151771
C84	6.4468838895	2.1185750760	14.6203983019
C85	6.7357675758	3.8485987432	12.9708523985
H86	2.2693818234	0.2301836809	12.1092690576
C87	2.6629289668	1.8632895345	10.6899129264
H88	3.6269567327	3.2927136782	9.3232365578
C89	6.3013807346	3.0923264802	15.6110898519
H90	6.4087851822	1.0631665401	14.8901307672
H91	6.9361566929	4.1567108269	11.9449596767
C92	6.5818876419	4.8183187076	13.9565585723
C93	1.2987498155	2.1426585408	10.3246241932

C94	6.3401557570	4.4523213244	15.2870750945
H95	6.1593200666	2.7876954397	16.6484376966
H96	6.6604488038	5.8719362957	13.6897460101
C97	0.1931328115	1.4261985657	10.8763170692
C98	0.9461051619	3.1699963069	9.4030761509
C99	6.0394957025	5.5107433021	16.3212084575
H100	0.3353169620	0.5708238113	11.5288957466
C101	-1.0961145598	1.7800600271	10.5968523446
C102	-0.3644408259	3.4928603001	9.1583379093
H103	1.6968700472	3.7513516730	8.8768591460
N104	4.6137840582	5.9087003508	16.2430893633
H105	6.6381663693	6.4141906068	16.1700752930
H106	6.2258113533	5.1480283861	17.3364858494
N107	-1.3898383961	2.8300556667	9.7669373454
H108	-1.9450959710	1.2457857683	11.0121982394
H109	-0.6519258978	4.2811167632	8.4681868017
C110	3.6564477656	5.1073619480	16.8039103921
C111	4.2118325162	6.9164701397	15.4032234911
C112	-2.7979751437	3.2773220603	9.6111773585
C113	2.3296245698	5.2633325937	16.5186946126
H114	4.0272012695	4.3497464724	17.4906864180
H115	5.0052004617	7.5507915485	15.0164857397
C116	2.8958937398	7.1076486497	15.0903196110
H117	-3.3485194934	2.4833448355	9.0938481215
H118	-2.7805670763	4.1519719402	8.9536591694
C119	-3.4357685449	3.5833530750	10.9462701977
C120	1.8643753842	6.2515758869	15.6015535948
H121	1.6367899231	4.5872026902	17.0137141729
H122	2.6637538752	7.9355869970	14.4266676733
C123	-4.2733957709	2.6318736303	11.5395687534
C124	-3.1950576125	4.7881935372	11.6188782855
C125	0.4954398135	6.3508498252	15.2011665584
H126	-4.4853729652	1.7014086044	11.0136848284
C127	-4.8477707907	2.8725447348	12.7842744287
C128	-3.7654791491	5.0399724289	12.8741655911
H129	-2.5839929536	5.5554085011	11.1386619460
C130	-0.5347652030	5.4805522043	15.6908193886
C131	0.0408230118	7.3066136277	14.2424103822
H132	-5.5024274747	2.1297364821	13.2331747165
C133	-4.5908731463	4.0683264838	13.4498500565
C134	-3.5248155292	6.3352508893	13.6151461408
C135	-1.8099131597	5.5256581264	15.2050330470
H136	-0.3337581751	4.7481709291	16.4674172168
H137	0.7110618265	8.0520096725	13.8213949824
C138	-1.2445905220	7.3044368626	13.7763902163
H139	-5.0520066540	4.2616650610	14.4177952666
N140	-2.1746628899	6.4084521579	14.2197139722
H141	-4.2594463114	6.4545932116	14.4195398434

H142	-3.6232551010	7.2022440314	12.9543349920
H143	-2.5992666258	4.8736586685	15.5676313975
H144	-1.5883445338	8.0086378408	13.0251266398

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N1	0.9663864430	5.3324066020	19.9750809403
C2	1.0932819448	4.0059057887	20.6491029452
C3	-0.2532090535	5.7472335688	19.5277348343
C4	2.0541770229	6.1166975728	19.7559675001
H5	2.1493293056	3.8862542598	20.9084567371
H6	0.5226733890	4.0601518540	21.5826275417
C7	0.5865579482	2.8860774009	19.7690541913
H8	-1.1003966196	5.1172984258	19.7817608393
C9	-0.3923400470	6.8978093833	18.7961513506
C10	1.9617265697	7.2803186060	19.0261098289
H11	2.9899410477	5.7707783408	20.1870823498
C12	-0.6929079240	2.3641432845	19.9935222172
C13	1.3618586421	2.3573003820	18.7271311573
H14	-1.3985178290	7.1621046536	18.4901589043
C15	0.7319908360	7.6996990426	18.4625057746
H16	2.8788951438	7.8462929528	18.8936303594
C17	-1.1911076705	1.3412917993	19.1909098283
H18	-1.2940836586	2.7503985732	20.8159585803
C19	0.8660728230	1.3312208071	17.9094242011
H20	2.3823881527	2.7189413761	18.5829375807
C21	0.6286402254	8.8459525825	17.5703423123
C22	-0.4175243071	0.8304904441	18.1519783297
H23	-2.1808707125	0.9341901911	19.3811606083
C24	1.6805479389	0.7441142543	16.7800201660
C25	-0.5969387893	9.2366579698	16.9737989038
C26	1.7560707608	9.6312117010	17.2129155859
H27	-0.8020036512	0.0180180398	17.5358617409
N28	1.7157052890	1.6339297386	15.5882835861
H29	1.2636658992	-0.2181720857	16.4627094621
H30	2.7202516462	0.5699468837	17.0741769687
H31	-1.5379266550	8.7579371507	17.2281722901
C32	-0.6457452452	10.2383883089	16.0350008050
C33	1.6592614582	10.6293246432	16.2752401782
H34	2.7302863219	9.4765164260	17.6651011055
C35	0.5580736487	1.9443702144	14.9256327932
C36	2.8758227117	2.2124087122	15.1719362433
N37	0.4762827237	10.9124853361	15.6617235129
H38	-1.5717841606	10.5437605138	15.5546540177
H39	2.5106760447	11.2390152391	15.9850038938
C40	0.5363697677	2.8679095711	13.9164305429
H41	-0.3296674638	1.4086386395	15.2500929572
H42	3.7733193745	1.9081562453	15.7018973231
C43	2.9062376053	3.1309322470	14.1548497532

C44	0.4530475335	11.7907274816	14.4572357202
C45	1.7184757751	3.5581864534	13.4950334443
H46	-0.4242033510	3.0538017861	13.4448780301
H47	3.8793922445	3.5476504552	13.9072697836
H48	-0.5301128051	12.2685270691	14.4180634148
H49	1.2069839021	12.5691516018	14.6107527257
C50	0.7361259011	10.9556605819	13.2275758025
C51	1.7086789349	4.6101606330	12.5153037572
C52	-0.2991430559	10.4901424222	12.4102103776
C53	2.0510428152	10.5717174036	12.9302048730
C54	0.5093646350	5.0859991613	11.9146334736
C55	2.8917705281	5.2903399227	12.0806089855
H56	-1.3236415572	10.8113188754	12.5979663850
C57	-0.0316964032	9.6209755859	11.3489088077
C58	2.3161129179	9.7003103560	11.8773416487
H59	2.8790972747	10.9656499565	13.5189261026
C60	0.5017434262	6.1534159498	11.0573515228
H61	-0.4505101876	4.6249714582	12.1339319890
H62	3.8760925031	4.9810467186	12.4214484616
C63	2.8386489337	6.3508675418	11.2156690150
H64	-0.8501305398	9.2789022751	10.7143439897
C65	1.2747318873	9.1939437303	11.0884071132
H66	3.3464689860	9.4207996287	11.6587754819
N67	1.6493595287	6.8071246378	10.7126375490
H68	-0.4082823116	6.5377296639	10.6011288279
H69	3.7276249210	6.8757588988	10.8741707465
C70	1.5607771983	8.1348110027	10.0484888042
H71	2.5107877354	8.3038841428	9.5325154196
H72	0.7707269261	8.0763185607	9.2927407925
N73	5.3190461126	1.4377844685	11.4998722372
C74	6.6506844509	1.4526564800	12.1685450390
C75	4.3116376543	0.6788662943	12.0106781610
C76	5.0499825614	2.3288699258	10.5057394425
C77	6.6331523571	2.4811851808	13.2780598544
H78	7.3944656409	1.6840982466	11.3996822011
H79	6.8429749463	0.4421818286	12.5406474998
H80	4.5933473332	-0.0544413213	12.7622557413
C81	3.0144924764	0.8388290989	11.5857343761
C82	3.7671707341	2.5302681332	10.0580578579
H83	5.9007642940	2.8618261772	10.0898853173
C84	6.4436566856	2.1076009879	14.6123388361
C85	6.7329310255	3.8449609658	12.9689786932
H86	2.2686425832	0.1868478729	12.0316015318
C87	2.6753532403	1.8226414123	10.6240331948
H88	3.6338030368	3.2479389390	9.2545341180
C89	6.3103312274	3.0772655508	15.6098243954
H90	6.4045900344	1.0515306863	14.8792851771
H91	6.9348532364	4.1583811517	11.9448910821

C92	6.5918861482	4.8106433484	13.9616421538
C93	1.2940682264	2.1135995447	10.2627978302
C94	6.3541525096	4.4387119564	15.2915909583
H95	6.1770342776	2.7674844057	16.6468430246
H96	6.6813693854	5.8647837529	13.7003589177
C97	0.2049799948	1.4102148927	10.8424874147
C98	0.9472599932	3.1368149919	9.3467171403
C99	6.0575882909	5.4946459015	16.3313281675
H100	0.3505802444	0.5584054789	11.4991626688
C101	-1.0916593178	1.7714884541	10.5764208105
C102	-0.3708726871	3.4655992506	9.1164212896
H103	1.6941305560	3.7064596329	8.8018339314
N104	4.6251754197	5.8848395512	16.2451036590
H105	6.6494998443	6.4021757638	16.1801114759
H106	6.2415868387	5.1337368585	17.3473328774
N107	-1.3825555707	2.8170380793	9.7493787669
H108	-1.9381697942	1.2457856144	11.0084225288
H109	-0.6642357519	4.2518584042	8.4251905869
C110	3.6724728093	5.0830526500	16.8054972755
C111	4.2256525952	6.8864570620	15.4020505052
C112	-2.8007908378	3.2629416839	9.5938342179
C113	2.3428898956	5.2325912100	16.5152546422
H114	4.0448466933	4.3285166881	17.4953848031
H115	5.0168427528	7.5243780165	15.0162375176
C116	2.9079772490	7.0680814196	15.0822089166
H117	-3.3389502976	2.4606094374	9.0771274548
H118	-2.7846619205	4.1356135674	8.9337148483
C119	-3.4327110200	3.5660833205	10.9324940192
C120	1.8791182889	6.2149922262	15.5942855900
H121	1.6543245297	4.5492271186	17.0069459138
H122	2.6740480146	7.8907579379	14.4147485783
C123	-4.2726551978	2.6157373589	11.5253945559
C124	-3.1924379520	4.7728665866	11.6047122606
C125	0.5050505783	6.3186575120	15.1885632676
H126	-4.4879145864	1.6853429585	11.0007574932
C127	-4.8499020659	2.8600923727	12.7683389370
C128	-3.7620999834	5.0244857859	12.8611227910
H129	-2.5894130668	5.5439832663	11.1206172669
C130	-0.5284540916	5.4589324672	15.6838458784
C131	0.0584327250	7.2668874135	14.2227551903
H132	-5.5097443579	2.1205082530	13.2148450247
C133	-4.5908827333	4.0547739094	13.4353306451
C134	-3.5206540526	6.3188103570	13.6036378837
C135	-1.8054161982	5.5080720984	15.1971447836
H136	-0.3306865705	4.7303079966	16.4648840708
H137	0.7325445989	8.0029526304	13.7895812209
C138	-1.2300370472	7.2705088231	13.7571713413
H139	-5.0553244062	4.2488901245	14.4016400980

N140	-2.1643798698	6.3876432502	14.2096300790
H141	-4.2495639195	6.4387084050	14.4126276238
H142	-3.6167233720	7.1889955153	12.9467485993
H143	-2.5988890747	4.8640130588	15.5653621774
H144	-1.5685264015	7.9715600010	13.0002644438

mHo⁶⁺ -3217.60421810343

N1	0.7476545100	5.7046546363	20.2760243360
C2	0.7281730966	4.3029818272	20.8144328265
C3	-0.4120789872	6.3950808675	20.1454692718
C4	1.9122472834	6.2473009315	19.8486953151
H5	1.7547126194	4.0646204359	21.1036622746
H6	0.1223482445	4.3307584718	21.7266351355
C7	0.1488895136	3.3411353335	19.7992472405
H8	-1.3026007765	5.9505751307	20.5814500653
C9	-0.4484758186	7.5997302495	19.4735484634
C10	1.9277652520	7.4574468071	19.1835046685
H11	2.8164862115	5.6794993827	20.0524864647
C12	-1.2394766390	3.1651804362	19.7616955186
C13	0.9561373872	2.6075081212	18.9156409337
H14	-1.4096339981	8.1010876615	19.3994200053
C15	0.7275423519	8.1418270461	18.9202047774
H16	2.8914329080	7.8277188661	18.8434459153
C17	-1.8134219056	2.2664995293	18.8666390662
H18	-1.8746757052	3.7004787388	20.4654821463
C19	0.3839364854	1.7051169594	18.0028798120
H20	2.0426885914	2.7085102829	18.9670063705
C21	0.7047545538	9.3191017102	18.0254502997
C22	-1.0056142833	1.5393840861	17.9966541941
H23	-2.8879954942	2.1107320003	18.8705443617
C24	1.2164205399	0.9113774775	17.0186550910
C25	-0.4780218598	9.7030263067	17.3665034121
C26	1.8691968328	10.0466182541	17.7205661857
H27	-1.4549417649	0.7913237401	17.3451458376
N28	1.3729315654	1.6309896269	15.7192454075
H29	0.7537965728	-0.0580710985	16.8077949367
H30	2.2263251455	0.7198344371	17.3916405042
H31	-1.4379172786	9.2459567513	17.5862755508
C32	-0.4437965243	10.6578615380	16.3692575248
C33	1.8536744178	10.9972573922	16.7184490702
H34	2.8028106086	9.8983730709	18.2551034702
C35	0.2871373189	1.9052180198	14.9334697358
C36	2.5824342334	2.1457998529	15.3558896305
N37	0.7220358418	11.2505709436	16.0188538822
H38	-1.3311634388	10.9560190180	15.8165946320
H39	2.7386262395	11.5610911956	16.4373260494
C40	0.3598619602	2.8007724271	13.8998243686
H41	-0.6261758523	1.3719101871	15.1804942331

H42	3.4300533099	1.8241244072	15.9547550995
C43	2.7078436049	3.0219677886	14.3090724662
C44	0.7914191539	12.0615372115	14.7578592628
C45	1.5763635599	3.4798270764	13.5762240849
H46	-0.5505828729	2.9722382061	13.3326582247
H47	3.7069351218	3.3934341256	14.1025666380
H48	-0.1544264326	12.6028015941	14.6708606596
H49	1.5958421406	12.7895993154	14.8917856754
C50	1.0391252499	11.1376944444	13.5840362486
C51	1.6567823609	4.5542488254	12.6171085275
C52	-0.0170962835	10.6788868330	12.7894474709
C53	2.3376684217	10.6931176017	13.3019444652
C54	0.5121860421	5.0988914466	11.9660340325
C55	2.8800590634	5.2185201449	12.2946294103
H56	-1.0317623882	11.0304414441	12.9742681748
C57	0.2179816873	9.7761876684	11.7497083585
C58	2.5698094266	9.7876947464	12.2685932141
H59	3.1803390447	11.0635751844	13.8852101593
C60	0.5845884954	6.2367631333	11.2033391038
H61	-0.4723061635	4.6515050197	12.0733638526
H62	3.8334146369	4.8496443167	12.6574754852
C63	2.9089502953	6.3541014669	11.5284339348
H64	-0.6149175058	9.4509789931	11.1265933448
C65	1.5096169277	9.3026083073	11.4906242680
H66	3.5919020416	9.4781601072	12.0504772785
N67	1.7639806650	6.8972303735	11.0119129478
H68	-0.2851132890	6.6778411149	10.7202935359
H69	3.8310264744	6.8772135213	11.2855190997
C70	1.7592323762	8.2630794270	10.4183683231
H71	2.7261448795	8.4084877466	9.9270986897
H72	0.9824868977	8.2801580714	9.6473917345
N73	5.4163417741	1.4876203120	10.9194262389
C74	6.7591596128	1.6154586694	11.5791198852
C75	4.4993116183	0.6395839749	11.4429137482
C76	5.0851372846	2.3030551677	9.8892235890
C77	6.6521968929	2.5910286305	12.7329658312
H78	7.4625025708	1.9460402559	10.8090271394
H79	7.0513809111	0.6131546406	11.9056961298
H80	4.8438345151	-0.0327496767	12.2250648411
C81	3.1897905247	0.6617480362	11.0081436633
C82	3.7859095935	2.3614501569	9.4219825410
H83	5.8831199261	2.9100836529	9.4689888425
C84	6.4464661624	2.1388555312	14.0419563597
C85	6.7344743943	3.9705009333	12.5022786858
H86	2.4945470045	-0.0200779158	11.4885992358
C87	2.7818599971	1.5743967664	10.0163352248
H88	3.5829096499	3.0285424496	8.5883732967
C89	6.2970256865	3.0486183217	15.0919404009

H90	6.4099739167	1.0699928033	14.2499093941
H91	6.9345603988	4.3453842979	11.4991032559
C92	6.5771279593	4.8769891084	13.5499732829
C93	1.3497663021	1.7536579169	9.6947721322
C94	6.3363813930	4.4280761294	14.8558336171
H95	6.1624924026	2.6754689182	16.1073075161
H96	6.6733130599	5.9440692197	13.3512452540
C97	0.3783777949	0.8028661183	10.0589948204
C98	0.8828145001	2.9395149984	9.1005127941
C99	6.0779655333	5.4181060237	15.9726084708
H100	0.6422619965	-0.1837665975	10.4289245471
C101	-0.9635463121	1.1038033037	9.9487665877
C102	-0.4723166515	3.1959625167	9.0095745876
H103	1.5597956761	3.7004799854	8.7286169007
N104	4.6373070806	5.7966579330	16.0086387650
H105	6.6488160715	6.3426470077	15.8391905899
H106	6.3276515121	5.0029289217	16.9536783107
N107	-1.3760770500	2.3085328143	9.4812394621
H108	-1.7361618115	0.4020574882	10.2424352634
H109	-0.8694748811	4.1116961816	8.5793428837
C110	3.7386621948	5.0270470019	16.6908926247
C111	4.1655763103	6.8022848608	15.2092795506
C112	-2.8316051554	2.6822367547	9.5666330649
C113	2.3870609105	5.1734786994	16.5101821219
H114	4.1652483523	4.2911169437	17.3697485233
H115	4.9219376087	7.4366270933	14.7530589537
C116	2.8237564137	6.9865104818	15.0065219133
H117	-3.3946041672	1.8499797041	9.1335038872
H118	-2.9678933134	3.5558215074	8.9248566877
C119	-3.2457067925	2.9393879920	11.0000606556
C120	1.8469487538	6.1245996499	15.5961924334
H121	1.7362777967	4.5110278377	17.0758385366
H122	2.5350563217	7.8058418372	14.3546988702
C123	-3.7654894571	1.8819164758	11.7535128362
C124	-3.1383972366	4.2096788438	11.5894200469
C125	0.4481407628	6.1794528440	15.2600632133
H126	-3.8825880774	0.8989798963	11.3000555715
C127	-4.1752234087	2.0870964074	13.0677795661
C128	-3.5572185814	4.4280652657	12.9126523735
H129	-2.7758830185	5.0437533332	10.9856660106
C130	-0.5123527310	5.2503234893	15.7633756946
C131	-0.0861762760	7.1279107215	14.3402888362
H132	-4.6033221028	1.2653507702	13.6337422859
C133	-4.0765623059	3.3512038083	13.6413635629
C134	-3.4989490177	5.7929796996	13.5636586922
C135	-1.7786982116	5.1842540839	15.2512764380
H136	-0.2596267870	4.5370171596	16.5434641702
H137	0.5123566053	7.9510694078	13.9611512998

C138	-1.3686949827	7.0322630586	13.8668037712
H139	-4.4578411719	3.5156706810	14.6462650410
N140	-2.2033748391	6.0320932607	14.2646475298
H141	-4.3030884999	5.9027967138	14.2986020911
H142	-3.6114303510	6.5976102117	12.8338519016
H143	-2.5096924015	4.4629372305	15.6000185755
H144	-1.7873227940	7.7395918736	13.1548660377

mHo⁷⁺ -3217.40679997866

N1	0.0724977820	5.6492587073	20.2429392934
C2	-0.1363638089	4.2233722938	20.6810267885
C3	-1.0054777416	6.4323053516	19.9918670098
C4	1.3212567033	6.1314813760	20.0417231161
H5	0.8041813162	3.8913146379	21.1300030387
H6	-0.8967902319	4.2494311678	21.4684304269
C7	-0.5713196897	3.3425461758	19.5221973085
H8	-1.9800567853	6.0304003131	20.2570306260
C9	-0.8599675920	7.6765530917	19.4092410414
C10	1.5177357116	7.3700909428	19.4530143341
H11	2.1468389464	5.4926013276	20.3486111241
C12	-1.9364754622	3.2352182694	19.2220366459
C13	0.3548956112	2.6074883403	18.7595735384
H14	-1.7662051391	8.2512305212	19.2377263102
C15	0.4168939648	8.1519270402	19.0538055169
H16	2.5453072655	7.6879634699	19.2993719373
C17	-2.3749807588	2.3911463642	18.2020744464
H18	-2.6697891153	3.7800733665	19.8160703913
C19	-0.0799994698	1.7442230359	17.7382538050
H20	1.4175627312	2.6529637977	19.0096571380
C21	0.5898990736	9.3420850242	18.1811743205
C22	-1.4540311561	1.6307185396	17.4848014874
H23	-3.4378013316	2.2886361919	17.9844267393
C24	0.8899607767	0.9399228716	16.8944336704
C25	-0.5018064735	9.8806880148	17.4750222057
C26	1.8532866944	9.9070746023	17.9253863351
H27	-1.8114110016	0.9082512887	16.7510256146
N28	1.2080793809	1.6827159070	15.6247674035
H29	0.4591309780	-0.0218860391	16.5944179850
H30	1.8413934580	0.7489947659	17.3987007274
H31	-1.5240369820	9.5563618597	17.6455557966
C32	-0.3026909343	10.8264137096	16.4863756814
C33	2.0055934231	10.8462460038	16.9202918861
H34	2.7437946892	9.6284896289	18.4835731043
C35	0.2070793190	1.9526529891	14.7448036177
C36	2.4521006858	2.1651137889	15.3799239850
N37	0.9451466966	11.2519459290	16.1807192743
H38	-1.1231186563	11.2445849078	15.9072594436
H39	2.9710950303	11.2834449876	16.6754779697

C40	0.3865274496	2.8231171848	13.6971304217
H41	-0.7402912110	1.4583456812	14.9315341082
H42	3.2303088152	1.8536274712	16.0750444509
C43	2.6839224696	3.0316361774	14.3295400505
C44	1.1666333532	12.0657774934	14.9354124550
C45	1.6325384375	3.4669723055	13.4869423248
H46	-0.4754879913	3.0075851125	13.0626834612
H47	3.6996428838	3.3952831987	14.2094191890
H48	0.2799128729	12.6942857841	14.8073699739
H49	2.0251474947	12.7163650604	15.1263249713
C50	1.3925625757	11.1435627174	13.7516409863
C51	1.7831142497	4.5783047740	12.5476914425
C52	0.3101810689	10.6393455370	13.0154801967
C53	2.6893795203	10.7679509916	13.3756864592
C54	0.6764223886	5.1291650462	11.8520658113
C55	3.0219540946	5.2281772175	12.3210605343
H56	-0.7061006432	10.9556804786	13.2508469284
C57	0.5178722393	9.7581139404	11.9521780270
C58	2.8972559685	9.8859729560	12.3118972393
H59	3.5508162263	11.1830955642	13.8986218280
C60	0.7915209627	6.2962085194	11.1264859215
H61	-0.3076111015	4.6706954972	11.9067876905
H62	3.9508135735	4.8508308994	12.7387279930
C63	3.0914742097	6.3933065695	11.5902678972
H64	-0.3395574514	9.4110514062	11.3743491718
C65	1.8139154825	9.3553368324	11.5975612422
H66	3.9177177080	9.6344877363	12.0211999301
N67	1.9806734720	6.9488020378	11.0303478246
H68	-0.0492391831	6.7533745586	10.6061571049
H69	4.0257000225	6.9240378135	11.4161479773
C70	2.0404612924	8.3493322164	10.4849618915
H71	3.0255344870	8.4601486808	10.0214528920
H72	1.2795058344	8.4158970391	9.7011147724
N73	5.3834866988	1.5830130772	10.6726859233
C74	6.7557725151	1.8367284640	11.2348389504
C75	4.6009915386	0.6155756185	11.2062934725
C76	4.9000998915	2.3889103045	9.6975648518
C77	6.6823807418	2.8414074606	12.3693799843
H78	7.3764054784	2.1894309534	10.4058723953
H79	7.1440016854	0.8683321753	11.5655558060
H80	5.0638422483	-0.0498931178	11.9317338724
C81	3.2692397058	0.5056838684	10.8486721277
C82	3.5746313247	2.3168216712	9.3101163837
H83	5.5963636531	3.0973456494	9.2549454114
C84	6.4364032480	2.4195941824	13.6837180997
C85	6.8642724123	4.2096603494	12.1277863859
H86	2.6976941552	-0.2828112046	11.3301037868
C87	2.6982815863	1.4060300740	9.9296717322

H88	3.2552213162	2.9964208350	8.5250223778
C89	6.3548919097	3.3447955360	14.7258342933
H90	6.3423475602	1.3571135054	13.9086414653
H91	7.1002659099	4.5600769486	11.1231709398
C92	6.7818994475	5.1362081821	13.1705841142
C93	1.2266249197	1.4732076145	9.7240835165
C94	6.5130975723	4.7167450528	14.4801241978
H95	6.2050248404	2.9851418765	15.7446935395
H96	6.9585129754	6.1912661943	12.9609975071
C97	0.3490530526	0.5756170830	10.3626329086
C98	0.6316056491	2.5174260940	8.9922957234
C99	6.3765576977	5.7221049997	15.6085017368
H100	0.6927951742	-0.3178762851	10.8752644727
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C102	-0.7361550122	2.7251271799	9.0451765613
H103	1.2091501679	3.2158278433	8.3934017186
N104	4.9306077943	6.0828960677	15.7896815509
H105	6.9142829052	6.6530187919	15.4054626785
H106	6.7246402426	5.3224730891	16.5650137268
N107	-1.5312612816	1.9185583428	9.7846071741
H108	-1.7044570076	0.1525433637	10.8864290932
H109	-1.2214542547	3.5473088399	8.5240727463
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C113	2.7554822651	5.4121257285	16.4885916546
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H122	2.6448522012	8.0411939586	14.3406673649
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C124	-3.1178542663	3.9146346484	11.9765547275
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H126	-3.7601702527	0.5653626712	11.9644210980
C127	-3.8603796306	1.8385181595	13.6925638828
C128	-3.3798335504	4.1913111675	13.3296449013
H129	-2.8886729863	4.7358325634	11.2921699654
C130	-0.1806633123	5.3458766373	15.9210396347
C131	0.0817021285	7.1264642140	14.3533356301
H132	-4.1732014445	1.0318677915	14.3512662480
C133	-3.7395768124	3.1366017896	14.1817407079
C134	-3.3308828308	5.5972773080	13.8915670219
C135	-1.4695062295	5.1833209592	15.4773974411

H136	0.1443881583	4.6849630280	16.7199972906
H137	0.6302291869	7.9244459425	13.8612628778
C138	-1.2158863778	6.9251450020	13.9324748218
H139	-3.9451716145	3.3396241092	15.2354882071
N140	-1.9792802305	5.9323353198	14.4593095477
H141	-4.0522781403	5.7165422708	14.7075582792
H142	-3.5502776094	6.3586549221	13.1371067477
H143	-2.1342884495	4.4402262505	15.9059072643
H144	-1.6943982488	7.5375303311	13.1696970383

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N1	-0.0647675809	5.7614811135	20.2102468471
C2	-0.2958715906	4.3437428366	20.6736815950
C3	-1.1291258458	6.5446837043	19.9013904348
C4	1.1918726523	6.2467380603	20.0704000823
H5	0.6264547791	4.0229276181	21.1671115681
H6	-1.0850563574	4.3925716110	21.4314199095
C7	-0.6892936439	3.4111339679	19.5352647694
H8	-2.1166056227	6.1483932687	20.1263261693
C9	-0.9553406466	7.7874721034	19.3198793119
C10	1.4159700157	7.4817725920	19.4812350930
H11	2.0033290003	5.6159395548	20.4289790110
C12	-2.0462628951	3.2723524763	19.2061831656
C13	0.2604835513	2.6335665114	18.8427857284
H14	-1.8536140938	8.3614902137	19.1057782686
C15	0.3372723294	8.2626285970	19.0220676085
H16	2.4506978634	7.8010392217	19.3843899574
C17	-2.4552659683	2.3562951179	18.2361405590
H18	-2.7992753120	3.8479751278	19.7440861940
C19	-0.1491049353	1.6870988968	17.8825998636
H20	1.3153865126	2.6931200519	19.1227352638
C21	0.5530405204	9.4381881280	18.1344255453
C22	-1.5157933422	1.5436264056	17.6040306866
H23	-3.5101916860	2.2429063894	17.9892848058
C24	0.8429704294	0.8164393717	17.1338667786
C25	-0.5100396605	9.9813267651	17.3872664277
C26	1.8337824443	9.9728205755	17.8932436686
H27	-1.8546137667	0.7614479700	16.9232787991
N28	1.1986898907	1.4931587883	15.8199717856
H29	0.4148054843	-0.1555881862	16.8629649012
H30	1.7816301536	0.6509306647	17.6707192274
H31	-1.5448980418	9.6933886215	17.5495088617
C32	-0.2687129488	10.8882910026	16.3707480127
C33	2.0299736465	10.8682463525	16.8543323498
H34	2.7064780426	9.6967597605	18.4804127350
C35	0.2187933181	1.7047088015	14.9106421216
C36	2.4412208935	1.9636040801	15.5880289011
N37	0.9967195939	11.2663048081	16.0712254674

H38	-1.0684648598	11.3118878781	15.7659557286
H39	3.0114357484	11.2733177520	16.6153567889
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H41	-0.7312600252	1.2140187629	15.1010886755
H42	3.2086547565	1.6897802013	16.3135159047
C43	2.6846957831	2.8054704106	14.5079880391
C44	1.2674450728	12.0101485648	14.7907685483
C45	1.6511321334	3.1866579958	13.6347359812
H46	-0.4309678234	2.6855209007	13.1623765146
H47	3.6989641331	3.1797663278	14.4015127174
H48	0.4046644976	12.6602399676	14.6123628130
H49	2.1436161598	12.6421022867	14.9635829018
C50	1.4855019936	11.0227623117	13.6549611388
C51	1.8125403493	4.3102850524	12.6652818721
C52	0.3992136014	10.4562710975	12.9670394027
C53	2.7832423500	10.6566518181	13.2698440739
C54	0.7232039573	4.8473300394	11.9493413989
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H56	-0.6195499828	10.7725159690	13.1933858281
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C58	2.9913431530	9.7152224844	12.2566883274
H59	3.6460716526	11.1232722975	13.7452444588
C60	0.8545717100	6.0142531726	11.2052742419
H61	-0.2645158918	4.3923907493	11.9847566170
H62	3.9715946388	4.5847200290	12.9111420097
C63	3.1326544658	6.1218338225	11.7257802825
H64	-0.2559782402	9.1334840423	11.4033487685
C65	1.9049446295	9.1183920729	11.6018188836
H66	4.0121033520	9.4758759919	11.9557641383
N67	2.0388566468	6.6693723609	11.1450041574
H68	0.0271740254	6.4620862937	10.6518328877
H69	4.0682992124	6.6613397852	11.5811277010
C70	2.1346040591	8.0648053654	10.5376662738
H71	3.1329248465	8.1291131386	10.0928876355
H72	1.3908424505	8.1048226828	9.7355754314
N73	5.3447484746	1.8002979688	10.4630983981
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C75	4.5982252960	0.7817851944	10.9541642656
C76	4.8361283061	2.6104220844	9.5027361655
C77	6.6327583324	3.0290344656	12.2258775845
H78	7.3126842824	2.4938734242	10.2233774720
H79	7.1323888043	1.1136879088	11.3181539084
H80	5.0849091799	0.1039774641	11.6528143050
C81	3.2728956508	0.6307984587	10.5831537619
C82	3.5155729863	2.4989490786	9.1041099652
H83	5.5109840610	3.3496681280	9.0761184163
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C85	6.8367136070	4.4081382524	12.0662999212

H86	2.7344945959	-0.2027024837	11.0267192282
C87	2.6675996947	1.5418959827	9.6956226811
H88	3.1768556312	3.1821077264	8.3292155830
C89	6.3309681768	3.4072581680	14.6154772506
H90	6.3081348551	1.4671165169	13.6932241513
H91	7.0894571399	4.8114985662	11.0856453906
C92	6.7817400820	5.2771093946	13.1626362845
C93	1.1883808770	1.5893167174	9.5200902076
C94	6.5118943040	4.7904710444	14.4503924017
H95	6.1967875537	2.9875265176	15.6141901466
H96	6.9888241203	6.3367501822	13.0098154130
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C99	6.4255457452	5.7283946051	15.6456826331
H100	0.7034649066	-0.2164397949	10.6723635471
C101	-1.0220147702	0.9162492076	10.2521523096
C102	-0.8059136900	2.8397563643	8.9288169327
H103	1.1095385935	3.3365093306	8.1945005355
N104	4.9720160454	6.1008972461	15.8679282755
H105	6.9691421897	6.6658517632	15.4910586038
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H108	-1.6942135097	0.2374528913	10.7712402617
H109	-1.3149111131	3.6626400650	8.4302990851
C110	4.1834027089	5.3044141602	16.6233653290
C111	4.4275431692	7.1297811323	15.1777464663
C112	-2.9971133075	2.3928398385	10.0152964310
C113	2.8021263735	5.4336180342	16.5780610687
H114	4.6875476272	4.5591343780	17.2406094467
H115	5.1280686955	7.7990186465	14.6771471506
C116	3.0513553148	7.2893863450	15.1067481233
H117	-3.6121500950	1.5441159636	9.6970632066
H118	-3.2487583366	3.2489873651	9.3828649300
C119	-3.1883944899	2.6814046495	11.4953377289
C120	2.1816812781	6.3835650203	15.7443457816
H121	2.2259424851	4.7363054326	17.1799687410
H122	2.6848413517	8.1155942074	14.5022026219
C123	-3.5600297193	1.6285383001	12.3424317185
C124	-3.0723082469	3.9789660575	12.0338717772
C125	0.7155449538	6.3340235822	15.4420227805
H126	-3.7088566755	0.6284393226	11.9356462242
C127	-3.7911838045	1.8503260030	13.6987755307
C128	-3.3267722436	4.2140332929	13.3997823482
H129	-2.8646553727	4.8221328497	11.3695858253
C130	-0.1399051900	5.3882901422	16.0423425214
C131	0.1160698726	7.1503834365	14.4652170631
H132	-4.0993621973	1.0229521365	14.3332705458
C133	-3.6790886916	3.1348556409	14.2256614146

C134	-3.3094938590	5.6054241199	14.0006088936
C135	-1.4372367404	5.2182531876	15.5949555150
H136	0.1842131650	4.7353139479	16.8496228206
H137	0.6626822716	7.9436482166	13.9638987660
C138	-1.1915700981	6.9404631523	14.0374780202
H139	-3.9055893421	3.3060110691	15.2818069244
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H142	-3.5427039175	6.3917216997	13.2771789292
H143	-2.1015210130	4.4733323934	16.0243177147
H144	-1.6720401308	7.5442238840	13.2659787737

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